METHODS OF MODERN MATHEMATICAL PHYSICS

III: SCATTERING THEORY

MICHAEL REED

Department of Mathematics
Duke University

BARRY SIMON

Departments of Mathematics
and Physics
Princeton University

ACADEMIC PRESS, INC.
Harcourt Brace Jovanovich, Publishers
San Diego New York Berkeley Boston
London Sydney Tokyo Toronto

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ACADEMIC PRESS, INC.
1250 Sixth Avenue, San Diego, California 92101

United Kingdom Edition published by
ACADEMIC PRESS, INC. (LONDON) LTD.
24/28 Oval Road, London NW1 7DX

Library of Congress Cataloging in Publication Data

Reed, Michael.
Methods of modern mathematical physics.

Vol. 3 Scattering Theory.
Includes bibliographical references.
CONTENTS: v. 1. Functional analysis.–v. 2. Fourier analysis, self–adjointness.–v. 3. Scattering theory.–v. 4. Analysis of operators.
1. Mathematical physics. I. Simon, Barry, joint author. II. Title.
QC20.R37 1972 530.1'5 75–182650
ISBN 0–12–585003–4 (v. 3)

AMS (MOS) 1970 Subject Classifications: 47–02, 81–02

PRINTED IN THE UNITED STATES OF AMERICA

88 89 90 91 92 10 9 8 7 6 5

To Martha and Jackie

Scattering theory is the study of an interacting system on a scale of time and/or distance which is large compared to the scale of the interaction itself. As such, it is the most effective means, sometimes the only means, to study microscopic nature. To understand the importance of scattering theory, consider the variety of ways in which it arises. First, there are various phenomena in nature (like the blue of the sky) which are the result of scattering. In order to understand the phenomenon (and to identify it as the result of scattering) one must understand the underlying dynamics and its scattering theory. Second, one often wants to use the scattering of waves or particles whose dynamics one knows to determine the structure and position of small or inaccessible objects. For example, in x-ray crystallography (which led to the discovery of DNA), tomography, and the detection of underwater objects by sonar, the underlying dynamics is well understood. What one would like to construct are correspondences that link, via the dynamics, the position, shape, and internal structure of the object to the scattering data. Ideally, the correspondence should be an explicit formula which allows one to reconstruct, at least approximately, the object from the scattering data. A third use of scattering theory is as a probe of dynamics itself. In elementary particle physics, the underlying dynamics is not well understood and essentially all the experimental data are scattering data. The main test of any proposed particle dynamics is whether one can construct for the dynamics a scattering theory that predicts the observed experimental data. Scattering theory was not always so central to physics. Even though the Coulomb cross section could have been computed by Newton, had he bothered to ask the right question, its calculation is generally attributed to Rutherford more than two hundred years later. Of course, Rutherford's calculation was in connection with the first experiment in nuclear physics.

Scattering theory is so important for atomic, condensed matter, and high energy physics that an enormous physics literature has grown up. Unfortunately, the development of the associated mathematics has been much slower. This is partially because the mathematical problems are hard but also because lack of communication often made it difficult for mathematicians to appreciate the many beautiful and challenging problems in scattering theory. The physics literature, on the other hand, is not entirely satisfactory because of the many heuristic formulas and ad hoc methods. Much of the physics literature deals with the "time-independent" approach to scattering theory because the time-independent approach provides powerful calculational tools. We feel that to use the time-independent formulas one must understand them in terms of and derive them from the underlying dynamics. Therefore, in this book we emphasize scattering theory as a time-dependent phenomenon, in particular, as a comparison between the interacting and free dynamics. This approach leads to a certain imbalance in our presentation since we therefore emphasize large times rather than large distances. However, as the reader will see, there is considerable geometry lurking in the background.

The scattering theories in branches of physics as different as classical mechanics, continuum mechanics, and quantum mechanics, have in common the two foundational questions of the existence and completeness of the wave operators. These two questions are, therefore, our main object of study in individual systems and are the unifying theme that runs throughout the book. Because we treat so many different systems, we do not carry the analysis much beyond the construction and completeness of the wave operators, except in two-body quantum scattering, which we develop in some detail. However, even there, we have not been able to include such important topics as Regge theory, inverse scattering, and double dispersion relations.

Since quantum mechanics is a linear theory, it is not surprising that the heart of the mathematical techniques is the spectral analysis of Hamiltonians. Bound states (corresponding to point spectra) of the interaction Hamiltonian do not scatter, while states from the absolutely continuous spectrum do. The mathematical property that distinguishes these two cases (and that connects the physical intuition with the mathematical formulation) is the decay of the Fourier transform of the corresponding spectral measures. The case of singular continuous spectrum lies between and the crucial (and often hardest) step in most proofs of asymptotic completeness is the proof that the interacting Hamiltonian has no singular continuous spectrum. Conversely, one of the best ways of showing that a self-adjoint operator has no singular continuous spectrum is to show that it is the interaction Hamiltonian of a quantum system with complete wave operators. This deep connection between scattering theory and spectral analysis shows the artificiality of the division of material into Volumes III and IV. We have, therefore, preprinted at the end of this volume three sections on the absence of continuous singular spectrum from Volume IV.

While we were reading the galley proofs for this volume, V. Enss introduced new and beautiful methods into the study of quantum-mechanical scattering. Enss's paper is not only of interest for what it proves, but also for the future direction that it suggests. In particular, it seems likely that the methods will provide strong results in the theory of multiparticle scattering. We have added a section at the end of this Chapter (Section XI.17) to describe Enss's method in the two-body case. We would like to thank Professor Enss for his generous attitude, which helped us to include this material.

The general remarks about notes and problems made in earlier introductions are applicable here with one addition: the bulk of the material presented in this volume is from advanced research literature, so many of the problems are quite substantial. Some of the starred problems summarize the contents of research papers!

Contents

Preface vii
Introduction ix
Contents of Other Volumes xv

XI: SCATTERING THEORY

1. *An overview of scattering phenomena* 1
2. *Classical particle scattering* 5
3. *The basic principles of scattering in Hilbert space* 16

Appendix 1 Stationary phase methods 37
Appendix 2 Trace ideal properties of $f(x)g(-i\nabla)$ 47
Appendix 3 A general invariance principle for wave operators 49

4. *Quantum scattering I: Two-body case* 54
5. *Quantum scattering II: N-body case* 75
6. *Quantum scattering III: Eigenfunction expansions* 96

Appendix Introduction to eigenfunction expansions by the auxiliary space method 112

7. *Quantum scattering IV: Dispersion relations* 116
8. *Quantum scattering V: Central potentials* 121
    - A. *Reduction of the S-matrix by symmetries* 121
    - B. *The partial wave expansion and its convergence* 127
    - C. *Phase shifts and their connection to the Schrödinger equation* 129
    - D. *The variable phase equation* 133
    - E. *Jost functions and Levinson's theorem* 136
    - F. *Analyticity of the partial wave amplitude for generalized Yukawa potentials* 143
    - G. *The Kohn variational principle* 147

Appendix 1 Legendre polynomials and spherical Bessel functions 149
Appendix 2 Jost solutions for oscillatory potentials 155
Appendix 3 Jost solutions and the fundamental problems of scattering theory 164
9. Long-range potentials 169
10. Optical and acoustical scattering I: Schrödinger operator methods 184
Appendix Trace class properties of Green's functions 203
11. Optical and acoustical scattering II: The Lax–Phillips method 210
Appendix The twisting trick 241
12. The linear Boltzmann equation 243
13. Nonlinear wave equations 252
Appendix Conserved currents 278
14. Spin wave scattering 285
15. Quantum field scattering I: The external field 293
16. Quantum field scattering II: The Haag–Ruelle theory 317
17. Phase space analysis of scattering and spectral theory 331
Appendix The RAGE theorem 340
Notes 344
Notes on scattering theory on C^*-algebras 382
Problems 385

MATERIAL PREPRINTED FROM VOLUME IV

XIII.6 The absence of singular continuous spectrum I: General theory 406
XIII.7 The absence of singular continuous spectrum II: Smooth perturbations 411
  A. Weakly coupled quantum systems 421
  B. Positive commutators and repulsive potentials 427
  C. Local smoothness and wave operators for repulsive potentials 433
XIII.8 The absence of singular continuous spectrum III: Weighted L^2 spaces 438
  Notes 447
  Problems 450

List of Symbols 455
Index 457

Contents of Other Volumes

Volume I: Functional Analysis

I *Preliminaries*
II *Hilbert Spaces*
III *Banach Spaces*
IV *Topological Spaces*
V *Locally Convex Spaces*
VI *Bounded Operators*
VII *The Spectral Theorem*
VIII *Unbounded Operators*

Volume II: Fourier Analysis, Self-Adjointness

IX *The Fourier Transform*
X *Self-Adjointness and the Existence of Dynamics*

Volume IV: Analysis of Operators

XII *Perturbation of Point Spectra*
XIII *Spectral Analysis*

Contents of Future Volumes: *Convex Sets and Functions, Commutative Banach Algebras, Introduction to Group Representations, Operator Algebras, Applications of Operator Algebras to Quantum Field Theory and Statistical Mechanics, Probabilistic Methods*

XI: Scattering Theory

It is notoriously difficult to obtain reliable results for quantum mechanical scattering problems. Since they involve complicated interference phenomena of waves, any simple uncontrolled approximation is not worth more than the weather forecast. However, for two body problems with central forces the computer can be used to calculate the phase shifts . . . . *W. Thirring*

XI.1 An overview of scattering phenomena

In this chapter we shall discuss scattering in a variety of physical situations. Our main goal is to illustrate the underlying similarities between the large time behavior of many kinds of dynamical systems. We study the case of nonrelativistic quantum scattering in great detail. Other systems we treat to a lesser extent, emphasizing simple examples.

Scattering normally involves a comparison of two different dynamics for the same system: the given dynamics and a "free" dynamics. It is hard to give a precise definition of "free dynamics" which will cover all the cases we consider, although we shall give explicit definitions in each individual case. The characteristics that these free dynamical systems have in common are that they are simpler than the given dynamics and generally they conserve the momentum of the "individual constituents" of the physical system. It is important to bear in mind that scattering involves more than just the interacting dynamics since certain features of the results will seem strange otherwise. Because two dynamics are involved, scattering theory can be viewed as a branch of perturbation theory. In the quantum-mechanical case we shall see that the perturbation theory of the absolutely continuous spectrum is involved rather than the perturbation theory of the discrete spectrum discussed in Chapter XII.

Scattering as a perturbative phenomenon emphasizes temporal asymptotics, and this is the approach we shall generally follow. But all the *concrete* examples we discuss will also have a geometric structure present and there is clearly lurking in the background a theory of scattering as correlations between spatial and temporal asymptotics. This is an approach we shall not explicitly develop, in part because it has been discussed to a much lesser degree. We do note that all the "free" dynamics we discuss have "straight-line motion" in the sense that solutions of the free equations which are concentrated as $t \to -\infty$ in some neighborhood of the direction $\mathbf{n}$ are concentrated as $t \to +\infty$ in a neighborhood of the direction $-\mathbf{n}$. These geometric ideas are useful for understanding the choice of free dynamics in Sections 14 and 16 where a piece of the interacting dynamics generates the free dynamics. And clearly, the geometric ideas are brought to the fore in the Lax–Phillips theory (Section 11) and in Enss's method (Section 17).

Scattering theory involves studying certain states of an interacting system, namely those states that appear to be "asymptotically free" in the distant past and/or the distant future. To be explicit, suppose that we can view the dynamics as transformations acting on the states. Let T_t and $T_t^{(0)}$ stand for the interacting and free dynamical transformations on the "set of states" Σ. Σ may be points in a phase space (classical mechanics), vectors in a Hilbert space (quantum mechanics), or Cauchy data for some partial differential equation (acoustics, optics). One is interested in pairs $\langle \rho_-, \rho \rangle \in \Sigma$ so that

$$\lim_{t \to -\infty} (T_t \rho - T_t^{(0)} \rho_-) = 0$$

for some appropriate sense of limit, and similarly for pairs that approach each other as $t \to +\infty$. One requirement that one must make on the notion of limit is that for each ρ there should be at most one ρ_-.

The basic questions of scattering theory are the following:

(1) *Existence of scattering states* Physically, one prepares the interacting system in such a way that some of the constituents are so far from one another that the interaction between them is negligible. One then "lets go," that is, allows the interacting dynamics to act for a long time and then looks at what has happened. One usually describes the initial state in terms of the variables natural to describe free states, often momenta. One expects that any free state "can be prepared," that is, for any $\rho_- \in \Sigma$, there is a $\rho \in \Sigma$ with $\lim_{t \to -\infty} T_t \rho - T_t^{(0)} \rho_- = 0$. Proving this is the basic existence question of scattering.

(2) *Uniqueness of scattering states* In order to describe the prepared state in terms of free states, one must know that each free state is associated with a unique interacting state; that is, given ρ_- there is at most one ρ such that $T_t^{(0)}\rho_- - T_t\rho \to 0$ as $t \to -\infty$. Notice that this is distinct from the requirement on the limit above that there should be at most one ρ_- for each ρ.

(3) *Weak asymptotic completeness* Suppose that one has an interacting state ρ that looked like a free state in the distant past in the sense that $\lim_{t\to-\infty} T_t^{(0)}\rho_- - T_t\rho = 0$ for some state ρ_-. One hopes that for large positive times, the interacting state will again look like a free state in the sense that there exists a state ρ_+ so that $\lim_{t\to+\infty} T_t^{(0)}\rho_+ - T_t\rho = 0$. In order to prove this, one needs to show that the two subsets of Σ

$$\Sigma_{\text{in}} = \left\{\rho \in \Sigma \,\middle|\, \exists\rho_- \in \Sigma \text{ with } \lim_{t\to-\infty} T_t^{(0)}\rho_- - T_t\rho = 0\right\}$$

and

$$\Sigma_{\text{out}} = \left\{\rho \in \Sigma \,\middle|\, \exists\rho_+ \in \Sigma \text{ with } \lim_{t\to+\infty} T_t^{(0)}\rho_+ - T_t\rho = 0\right\}$$

are equal. If in fact $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, then the system is said to have **weak asymptotic completeness**.

(4) *Definition of the S-transformation* If one has a pair of dynamical systems $\langle T_t^{(0)}, T_t\rangle$ for which one can prove existence and uniqueness of scattering states (both as $t \to -\infty$ and as $t \to \infty$) and for which weak asymptotic completeness holds, then one can define a natural bijection of Σ onto itself. Given $\rho \in \Sigma$, existence and uniqueness of scattering states assures us that there exists a state $\Omega^+\rho \in \Sigma_{\text{in}}$ with $\lim_{t\to-\infty} (T_t(\Omega^+\rho) - T_t^{(0)}\rho) = 0$. Similarly, Ω^- is defined by $\lim_{t\to+\infty} (T_t(\Omega^-\rho) - T_t^{(0)}\rho) = 0$. Ω^+ (respectively, Ω^-) is a bijection from Σ onto Σ_{in} (respectively, Σ_{out}). Weak asymptotic completeness assures us that $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, so one can define the *bijection*

$$S = (\Omega^-)^{-1}\Omega^+ : \Sigma \to \Sigma$$

S is called the **scattering transformation**. Thus, $T_t^{(0)}(S\rho)$ and $T_t^{(0)}\rho$ are related by the condition that there exists a state ψ ($\psi = \Omega^+\rho = \Omega^-(S\rho)$) so that $T_t\psi$ "interpolates" between them. That is, $T_t\psi$ looks like $T_t^{(0)}\rho$ in the past and $T_t^{(0)}S\rho$ in the future. Thus S correlates the past and future asymptotics of interacting histories. The reader should be warned that the maps $S' = \Omega^+(\Omega^-)^{-1}: \Sigma_{\text{in}} \to \Sigma_{\text{out}}$ and also the maps $(\Omega^+)^{-1}\Omega^-$ and $\Omega^-(\Omega^+)^{-1}$ occasionally appear in the literature. When weak asymptotic completeness holds, $S' = \Omega^- S(\Omega^-)^{-1}$, so S and S' are "similar." For this reason, the choice between S and S' is to some extent a matter of personal preference. We use S, the so-called EBFM S-matrix, throughout this book. We discuss the reasons for the $\pm$ convention in Sections 3 and 6.

In classical particle mechanics S is a bijection on phase space. In a quantum theory with weak asymptotic completeness S is a *linear* unitary transformation and is called the S-operator or occasionally the S-matrix.

(5) *Reduction of S due to symmetries* In many problems there is an underlying symmetry of *both* the free and interacting dynamics. This allows one to conclude a priori, without detailed dynamical calculations, that S has a special form. See Sections 2 and 8 for explicit details.

(6) *Analyticity and the S-transformation* A common refinement of scattering theory for wave phenomena (quantum theory, optics, acoustics) is the realization of S or the kernel of some associated integral operator as the boundary value of an analytic function. In a heuristic sense this analyticity is connected with Theorem IX.16. For schematically, S describes the response R of a system to some input I in the following form:

$$R(t) = \int_{-\infty}^{t} f(t - t')I(t')\, dt'$$

This formula has two features built in: (i) time translation invariance, that is, f is a function of only $t - t'$; (ii) causality: $R(t)$ depends only on $I(t')$ for $t' \leq t$. Thus f is a function on $[0, \infty)$. Its Fourier transform is thus the boundary value of an analytic function. It is this causality argument that is intuitively in the back of physicists' minds when discussing analytic properties. Unfortunately, the proofs of these properties do not go along such simple lines. We shall restrict our detailed discussion of analyticity to the two-body quantum-mechanical case (Section 7) and to the Lax–Phillips theory (Section 11).

(7) *Asymptotic completeness* Consider a system with forces between its components that fall off as the components are moved apart. Physically, one expects a state of such a system to "decay" into freely moving clusters or to remain "bound." In many situations, there is a natural set of bound states, $\Sigma_{\text{bound}} \subset \Sigma$. One can usually prove that $\Sigma_{\text{bound}} \cap \Sigma_{\text{in}} = \emptyset$. The above physical expectation is

$$\Sigma_{\text{bound}} \text{ "+" } \Sigma_{\text{in}} = \Sigma = \Sigma_{\text{bound}} \text{ "+" } \Sigma_{\text{out}} \tag{1}$$

" + " is different in classical and quantum-mechanical systems. In classical particle mechanics " + " indicates set theoretic union; in quantum theory it indicates a direct sum of Hilbert spaces. Establishing that (1) holds is the problem of proving **asymptotic completeness**. Notice that asymptotic completeness implies weak asymptotic completeness. We remark that implicit in the idea that each free state has an associated interacting state is the assumption that the free dynamics has no "bound" states.

We emphasize that the above description is schematic. In each physical theory there are complications, and various modifications must be made. Among these are: (i) In classical mechanics Σ comes equipped with sets of measure zero and the natural interpretation of statements like $\Sigma_{\text{in}} = \Sigma_{\text{out}}$ is that they differ by sets of measure zero. (ii) In some systems, including many-body systems, the state spaces of the free and interacting dynamics are different (see Sections 5, 15, and 16). (iii) In quantum-mechanical systems one can define an S-operator even without weak asymptotic completeness (see Section 4). Weak asymptotic completeness then becomes equivalent to the unitarity of S. (iv) In certain very special cases the free dynamics may have bound states (see Section 10). (v) In the Lax–Phillips theory (Section 11) the free dynamics is replaced by the geometric notion of "incoming" and "outgoing" subspaces.

Usually, the interacting dynamics is obtained initially by perturbing a simple dynamics which then plays the role of the "free" dynamics. However, in some special physical theories there is no natural unperturbed dynamics to compare with the interacting dynamics. In such cases one first isolates certain especially simple solutions of the interacting system. Then one tries to describe the asymptotic behavior of the complete interacting system in terms of the interactions of these simple solutions. Magnon scattering (Section 14) and the Haag–Ruelle theory (Section 16) are examples of such systems, as is the scattering theory for the Korteweg–deVries equation, which we do not treat.

XI.2 Classical particle scattering

The simplest system with which to illustrate the ideas of scattering theory is the classical mechanics of a single particle moving in an external force field $\mathbf{F}(\mathbf{r})$. This theory is equivalent to the scattering of two particles interacting with each other through a force field $\mathbf{F}(\mathbf{r}_1 - \mathbf{r}_2)$ because the center of mass motion of such a two-body system separates from the motion of $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$. We shall suppose that the particle has mass one, which is no loss of generality.

The states of such a single particle system are points in **phase space**, that is, a pair $\langle \mathbf{r}, \mathbf{v} \rangle \in \mathbb{R}^6$ representing the position and velocity of the particle. The free dynamical transformation is given by $T_t^{(0)}\langle \mathbf{r}, \mathbf{v} \rangle = \langle \mathbf{r} + \mathbf{v}t, \mathbf{v} \rangle$. Thus the free dynamics conserves the velocity. The interacting dynamics is given by $T_t\langle \mathbf{r}_0, \mathbf{v}_0\rangle = \langle \mathbf{r}(t), \mathbf{v}(t)\rangle$ where $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$ and $\mathbf{r}(t)$ solves the equation

$$\ddot{\mathbf{r}}(t) = \mathbf{F}(\mathbf{r}(t)) \tag{2a}$$

with initial conditions

$$\mathbf{r}(0) = \mathbf{r}_0, \qquad \dot{\mathbf{r}}(0) = \mathbf{v}_0 \tag{2b}$$

In order to be sure that (2) has a unique solution for all times, we shall suppose that

$$|\mathbf{F}(\mathbf{r})| \le C \qquad \text{for all } \mathbf{r} \tag{3a}$$

$$|\mathbf{F}(\mathbf{r}) - \mathbf{F}(\mathbf{r}')| \le D_R|\mathbf{r} - \mathbf{r}'| \qquad \text{if} \quad |\mathbf{r} - \mathbf{r}'| \le 1 \quad \text{and} \quad |\mathbf{r}| < R \tag{3b}$$

where D_R is an R-dependent constant. The techniques we developed in Section V.6 assure us that (2) has a unique solution for small time if (3b) holds, and it is not hard to prove that this solution exists for all times (see Proposition 1 in the appendix to Section X.1 and Problem 1). The only place where the conditions (3) enter in the theory that we shall develop is in establishing this global existence and uniqueness. If one can establish this by some other means, (3) can be dispensed with and conditions (4) below need be required to hold only for large distances. In particular, local repulsive singularities present no problem.

To establish the existence and uniqueness of scattering solutions, we shall need to have further restrictions on the forces. These restrictions, which require that the interaction between constituents falls off as $r \to \infty$, where $r = |\mathbf{r}|$, are typical of scattering theories. Specifically, we shall suppose that:

$$|\mathbf{F}(\mathbf{r})| \le Cr^{-\alpha} \qquad \text{for all } \mathbf{r} \text{ and some } \alpha > 2 \tag{4a}$$

$$|\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{y})| \le Dr^{-\beta}|\mathbf{x} - \mathbf{y}| \qquad \text{for all } \mathbf{x}, \mathbf{y} \text{ with } x, y \ge r \text{ and some } \beta > 2 \tag{4b}$$

Under these assumptions we shall prove the existence and uniqueness of scattering solutions. One can establish existence using only (4a) (Problem 2), but uniqueness requires the Lipschitz condition (4b) (Problem 3). This is reminiscent of the situation we encountered in Section V.6 when discussing solutions of differential equations with initial conditions. Lipschitz conditions were also required there for uniqueness. This is not surprising since according to our intuitive picture in Section 1, scattering solutions can be viewed as solutions obeying "initial conditions at $t = -\infty$."

The conditions (4) do not include the important case of Coulomb scattering where the theory must be modified. We discuss this case in Section 9.

Henceforth we shall drop the boldface notation for vectors except in the statements of theorems and in situations where confusion might arise between a vector and its length.

Theorem XI.1 (existence and uniqueness of scattering solutions; classical particles) Let $\mathbf{F}(\mathbf{r})$ be a function from $\mathbb{R}^3$ to $\mathbb{R}^3$ obeying (3) and (4). Let $\langle \mathbf{r}_{-\infty}, \mathbf{v}_{-\infty} \rangle \in \mathbb{R}^6$ be given with $\mathbf{v}_{-\infty} \neq 0$. Then there exists a unique solution of (2a) obeying

$$\lim_{t \to -\infty} |\dot{\mathbf{r}}(t) - \mathbf{v}_{-\infty}| = 0 \tag{5a}$$

and

$$\lim_{t \to -\infty} |\mathbf{r}(t) - \mathbf{r}_{-\infty} - \mathbf{v}_{-\infty} t| = 0 \tag{5b}$$

Proof Since we are assuming (3), by the above remarks it is sufficient to prove the existence and uniqueness of solutions in $(-\infty, T)$ for some T. In keeping with the idea that scattering solutions obey initial conditions at $t = -\infty$, it is natural to use the method of Section V.6.A and rewrite the differential equation as an integral equation. In fact, one can show (Problem 4) that $r(t)$ obeys (2a) and (5) on $(-\infty, T)$ if and only if $r(t) = r_{-\infty} + v_{-\infty} t + u(t)$, where u is continuous and satisfies

$$u(t) = \int_{-\infty}^{t} \int_{-\infty}^{s} F(r_{-\infty} + v_{-\infty}\tau + u(\tau))\, d\tau\, ds \tag{6}$$

where the integral converges absolutely.

Choose $T < 0$ so that:

(i) $|r_{-\infty} + v_{-\infty} t| \geq \frac{1}{2}|t|\,|v_{-\infty}|$ if $t < T$;
(ii) $C(\alpha - 1)^{-1}(\alpha - 2)^{-1}|\frac{1}{4}v_{-\infty}|^{-\alpha}|T|^{2-\alpha} < 1$;
(iii) $\gamma \equiv D(\beta - 1)^{-1}(\beta - 2)^{-1}|\frac{1}{4}v_{-\infty}|^{-\beta}|T|^{2-\beta} < 1$;
(iv) $\frac{1}{4}|T|\,|v_{-\infty}| > 1$.

Here C, α, D, β are the constants in condition (4). Now suppose that $u(t)$ is an $\mathbb{R}^3$-valued continuous function on $(-\infty, T)$ with $\|u\|_\infty \leq 1$. Let $r(t) = r_{-\infty} + v_{-\infty} t + u(t)$. (i) and (iv) assure us that $|r(t)| \geq \frac{1}{4}|t|\,|v_{-\infty}|$. By (4a), the integral $\int_{-\infty}^{t} \int_{-\infty}^{s} |F(r_{-\infty} + v_{-\infty}\tau + u(\tau))|\, d\tau\, ds$ converges absolutely.

Let

$$\mathscr{M}_T = \{u \in C(-\infty, T) \text{ with values in } \mathbb{R}^3 \mid \|u\|_\infty \leq 1\}$$

and define $\mathscr{F}: \mathscr{M}_T \to \mathscr{M}_T$ by

$$(\mathscr{F}u)(t) = \int_{-\infty}^{t} \int_{-\infty}^{s} F(r_{-\infty} + v_{-\infty}\tau + u(\tau))\, d\tau\, ds$$

(4a) and (ii) assure us that $\|\mathscr{F}u\|_\infty \le 1$ if $\|u\|_\infty \le 1$, so $\mathscr{F}$ maps the complete metric space $\mathscr{M}_T$ into itself. (4b) and (iii) imply that

$$\|\mathscr{F}u - \mathscr{F}v\|_\infty \le \gamma\|u - v\|_\infty$$

so $\mathscr{F}$ is a contraction on $\mathscr{M}_T$ since T was chosen to make $\gamma < 1$. Thus, by the contraction mapping principle (Theorem V.8), $\mathscr{F}$ has a unique fixed point in $\mathscr{M}_T$. It is easy to prove now that (6) has a unique solution. For if u_1 and u_2 both solve (6), then both will lie in $\mathscr{M}_{T'}$ for some $T' < T$. But by the above argument, there is a unique solution of (6) in $\mathscr{M}_{T'}$ for any $T' < T$, so $u_1 = u_2$ on $(-\infty, T')$. By the uniqueness of solutions with initial conditions at $-T' - 1$, $u_1 = u_2$ on $(-\infty, T)$. ▮

We now define two important maps:

Definition Let $\Sigma = \mathbb{R}^6$ and let $r_{a,b}^{(-\infty)}(t)$ be the solution of (2a) asymptotic to $a + bt$ at $-\infty$. Set $\Sigma_0 \equiv \Sigma\backslash\{\langle a, b\rangle \mid b = 0\}$. Then the **wave operator** $\Omega^+ : \Sigma_0 \to \Sigma$ is defined by

$$\Omega^+\langle a, b\rangle = \langle r_{a,b}^{(-\infty)}(0), \dot{r}_{a,b}^{(-\infty)}(0)\rangle$$

Similarly, Ω^- is defined by

$$\Omega^-\langle a, b\rangle = \langle r_{a,b}^{(+\infty)}(0), \dot{r}_{a,b}^{(+\infty)}(0)\rangle$$

Thus $\Omega^+ w$ is that point of phase space which is the $t = 0$ initial data for a solution of the interacting equations of motion which is asymptotic at $t = -\infty$ to the solution of the free equations of motion with data at $t = 0$ equal to w.

The wave operators have several important properties:

Theorem XI.2 Suppose that conditions (3) and (4) hold for a force field $\mathbf{F}(\mathbf{r})$ and let $\Omega^\pm$ be the associated wave operators. Then:

(a) Let T_t and $T_t^{(0)}$ be the interacting and free dynamics, respectively. Then for all $w \in \Sigma_0$,

$$\Omega^\pm w = \lim_{t \to \mp\infty} T_{-t} T_t^{(0)} w$$

where the limits are uniform on compact subsets of Σ_0.

(b) $\Omega^\pm T_s^{(0)} = T_s \Omega^\pm$ on Σ_0 for all s.

(c) (isometry of $\Omega^{\pm}$) If $\mathbf{F}$ is conservative, that is, if $\mathbf{F} = -\nabla V$ for some function V, then $\Omega^{\pm}$ are measure-preserving transformations.

(d) If $\mathbf{F}$ is conservative and $V(\mathbf{r}) \to 0$ as $r \to \infty$, then $E(\Omega^{\pm} w) = E_0(w)$ where $E(\mathbf{r}, \mathbf{v}) = \frac{1}{2}v^2 + V(\mathbf{r})$ and $E_0(\mathbf{r}, \mathbf{v}) = \frac{1}{2}v^2$.

(e) If $\mathbf{F}$ is C^{∞} and

$$\left| \frac{\partial^{|\alpha|} F(\mathbf{r})}{\partial r_1^{\alpha_1} \cdots \partial r_3^{\alpha_3}} \right| \le D_{\alpha} r^{-|\alpha| - 2 - \varepsilon}$$

for all $\mathbf{r}$, $\boldsymbol{\alpha}$ and some $\varepsilon > 0$, then $\Omega^{\pm}$ are C^{∞} maps.

Proof (a) This is a typical property of $\Omega^{\pm}$ and will be used to define the analogues of $\Omega^{\pm}$ in quantum-mechanical situations. Since $\Omega^{+} x = y$ means that $\lim_{t \to -\infty} |T_t y - T_t^{(0)} x| = 0$ and $(T_t)^{-1} = T_{-t}$, (a) is intuitively expected. We shall prove the formula for Ω^{+}; the proof is essentially identical for Ω^{-}. For fixed $T \in \mathbb{R}$, define $\mathcal{M}_T$ as before. For $\langle \mathbf{a}, \mathbf{b} \rangle \in \Sigma_0$, $t \le T$, and $u \in \mathcal{M}_T$, define the function $\mathscr{F}^{(t)}_{a,b,T} u$ on $(-\infty, T)$ by

$$(\mathscr{F}^{(t)}_{a,b,T} u)(s) = \int_t^s \int_t^{\sigma} F(a + b\tau + u(\tau))\, d\tau\, d\sigma$$

Let $\mathscr{F}^{(-\infty)}_{a,b,T} u$ be of the same form with $t = -\infty$. One now proves the following three facts (Problems 5, 6):

(i) For any compact $K \subset \Sigma_0$, we can find $T < 0$ so that for $\langle a, b \rangle \in K$ and $t \in (-\infty, T)$, $\mathscr{F}^{(t)}_{a,b,T}$ takes $\mathcal{M}_T$ into itself and is a contraction. The constant γ in the equation $\|\mathscr{F}^{(t)}_{a,b,T} u - \mathscr{F}^{(t)}_{a,b,T} v\|_{\infty} \le \gamma \|u - v\|_{\infty}$ may be chosen, independently of $\langle a, b \rangle \in K$ and $t \in (-\infty, T)$, to be less than 1.

(ii) If K and T are as defined in (i), for any $u \in \mathcal{M}_T$, $\lim_{t \to -\infty} \mathscr{F}^{(t)}_{a,b,T} u = \mathscr{F}^{(-\infty)}_{a,b,T} u$. The convergence is uniform on $\mathcal{M}_T$ and K.

(iii) A general result about contractions: Suppose that F_n form a family of maps of a complete metric space to itself. If $\rho(F_n p, F_n q) \le c\rho(p, q)$ for all p, q, n and some $c < 1$, if $\lim_{n \to \infty} F_n p = F_{\infty} p$ for all p, and if p_n (respectively, p_{∞}) are the unique fixed points of F_n (respectively, F_{∞}), then $\lim_{n \to \infty} p_n = p_{\infty}$. Moreover, the rate at which p_n converges to p_{∞} depends only on the rate at which $F_n p_{\infty}$ converges to $F_{\infty} p_{\infty} = p_{\infty}$ and c.

Let $u^{(t)}_{a,b,T}$ be the fixed point of $\mathscr{F}^{(t)}_{a,b,T}$. We conclude that $\lim_{t \to -\infty} u^{(t)}_{a,b,T} = u^{(-\infty)}_{a,b,T}$. Now, using the fact that T_{-T+1} is continuous from

Σ to Σ, we conclude the proof of (a):

$$\begin{aligned}\Omega^+\langle a, b\rangle &= T_{-T+1}\langle a + b(T-1) + u^{(-\infty)}_{a,b,T}(T-1), b + \dot{u}^{(-\infty)}_{a,b,T}(T-1)\rangle \\ &= \lim_{t\to-\infty} T_{-T+1}\langle a + b(T-1) + u^{(t)}_{a,b,T}(T-1), b + \dot{u}^{(t)}_{a,b,T}(T-1)\rangle \\ &= \lim_{t\to-\infty} T_{-T+1}T_{-t+T-1}T_t^{(0)}\langle a, b\rangle \\ &= \lim_{t\to-\infty} T_{-t}T_t^{(0)}\langle a, b\rangle\end{aligned}$$

(b) This is a general consequence of (a) since

$$\Omega^\pm T_s^{(0)}w = \lim_{t\to\mp\infty} T_{-t}T_{s+t}^{(0)}w = \lim_{\tau\to\mp\infty} T_{-\tau+s}T_\tau^{(0)}w = T_s\Omega^\pm w$$

Here we have used the continuity of T_s and the fact that as $t \to \pm\infty$, $\tau = s + t \to \pm\infty$ for fixed s.

(c) This is another general feature of scattering theory which we shall meet in quantum scattering in a slightly different guise. For conservative systems, it is known that T_t is measure-preserving (Theorem X.78). Similarly, $T_t^{(0)}$ is measure-preserving, so $T_{-t}T_t^{(0)}$ is measure-preserving for all t. Let f be a continuous function of compact support on Σ_0. Then, by (a),

$$\int f(\Omega^+ w)\, d^6w = \lim_{t\to-\infty} \int f(T_{-t}T_t^{(0)}w)\, d^6w = \int f(w)\, d^6w$$

Thus Ω^+, and similarly Ω^-, are measure-preserving maps.

(d) Follows from (a), the conservation of energy ($E \circ T_t = E$) and the assumption that $V \to 0$ as $r \to \infty$.

(e) Under the hypothesis, $\mathscr{F}^{(-\infty)}_{a,b,T}u$ is a C^∞ map of $\Sigma_0 \times \mathscr{M}_T$ into $\mathscr{M}_T$ (Problem 7). By a general theorem on smoothness of fixed points of contractions (Problem 5b) the fixed points of $\mathscr{F}^{(-\infty)}_{a,b,T}$ and hence their values at $t = T - 1$ are C^∞. Since T_t is a C^∞ mapping for each t, propagating the solution from $t = T - 1$ to $t = 0$, we conclude that $\Omega^\pm$ are C^∞ maps. ∎

The domains of $\Omega^\pm$ are all of Σ minus a set of measure 0. In general, the range of $\Omega^\pm$ will not be all of Σ or even Σ minus a set of measure zero.

Example Let F obey the hypotheses of (d) of Theorem XI.2. Then $\text{Ran}\,\Omega^+ \subseteq \{\langle a', b'\rangle \mid \frac{1}{2}|b'|^2 + V(a') > 0\}$. The set

$$\{\langle a', b'\rangle \mid \tfrac{1}{2}|b'|^2 + V(a') \le 0\}$$

has nonzero measure if V is continuous and negative at any point.

Definition Let $\Sigma_{\text{in}} = \operatorname{Ran}\Omega^+$, $\Sigma_{\text{out}} = \operatorname{Ran}\Omega^-$, and let Σ_{bound} be the set of $\langle \mathbf{r}, \mathbf{v}\rangle$ so that the solution $\mathbf{r}(t)$ of (2) satisfies

$$\sup_t |\mathbf{r}(t)| + \sup_t |\dot{\mathbf{r}}(t)| < \infty$$

Thus, bound states are those whose trajectories lie in bounded regions of phase space. Weak asymptotic completeness says that $\Sigma_{\text{in}} = \Sigma_{\text{out}}$, and asymptotic completeness that $\Sigma_{\text{in}} = \Sigma_{\text{out}} = \Sigma\backslash\Sigma_{\text{bound}}$. Since we have already thrown out sets of measure zero (namely, $\{\langle a, b\rangle \mid b = 0\}$) in defining $\Omega^\pm$, we should be prepared to have these equalities modulo sets of measure zero. In general, there do exist solutions that are asymptotically free as $t \to -\infty$ but not as $t \to +\infty$ (capture; see Problem 9).

If the force is conservative, that is, $\mathbf{F}(r) = -\nabla V(\mathbf{r})$, then by our hypotheses on $\mathbf{F}$, V is smooth and bounded. In this case, by conservation of energy, $|\dot{\mathbf{r}}(t)|$ is automatically bounded, so $\langle r, v\rangle \in \Sigma_{\text{bound}}$ if and only if $\sup_t |\mathbf{r}(t)| < \infty$.

Theorem XI.3 (asymptotic completeness; two-body classical particle scattering) Let $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ with $V \to 0$ as $r \to \infty$. Suppose also that $\mathbf{F}$ obeys (3) and (4). Then Σ_{in}, Σ_{out}, and $\Sigma\backslash\Sigma_{\text{bound}}$ agree up to sets of measure 0.

Proof Let $r_{q,v}(t)$ be the solution of $\ddot{r}(t) = F(r(t))$, $r(0) = q$, $\dot{r}(0) = v$. Define

$$N_\pm = \left\{ \langle q, v\rangle \;\middle|\; \overline{\lim_{t\to\pm\infty}}\, |r_{q,v}(t)| < \infty \right\}$$

We first want to show that N_+ and N_- agree up to sets of measure 0, that is, $\mu(N_+\backslash N_-) + \mu(N_-\backslash N_+) = 0$ where μ is Lebesgue measure. The measurability of sets like N_+, N_-, Σ_{bound} is left to Problem 10. Let $\{K_n\}$ be compact subsets of $\mathbb{R}^6$ with $\bigcup K_n = \mathbb{R}^6$, $K_n \subset K_{n+1}^{\text{int}}$. Let $N_+^{(n)} = \{\langle q, v\rangle \mid T_t\langle q, v\rangle \in K_n$ for all $t \in [0, \infty)\}$ and similarly for $N_-^{(n)}$. We first note that $N_\pm = \bigcup_n N_\pm^{(n)}$ for, using conservation of energy, if $\overline{\lim}_{t\to+\infty} |r_{q,v}(t)| < \infty$, then $T_t\langle q, v\rangle$ lies in a compact subset of $\mathbb{R}^6$ as t runs from 0 to ∞. Thus, if $p \in N_+\backslash N_-$, $p \in N_+^{(n)}\backslash N_-^{(n)}$ for some n. Therefore, it is sufficient to prove that $\mu(N_+^{(n)} \Delta N_-^{(n)}) = 0$ for each n. Let T_t be the interacting dynamics. We first note that $\bigcap_{k=1}^\infty T_k N_+^{(n)} \subset N_-^{(n)}$ and that $N_+^{(n)} \supset T_1 N_+^{(n)} \supset T_2 N_+^{(n)} \supset \cdots$. Thus

$$\mu(N_+^{(n)}\backslash N_-^{(n)}) \le \mu\left(N_+^{(n)} \middle\backslash \bigcap_{k=1}^{\infty} T_k N_+^{(n)} \right) \le \sum_{k=1}^{\infty} \mu(N_+^{(n)}\backslash T_k N_+^{(n)})$$

But, by Liouville's theorem, $\mu(T_k N_+^{(n)}) = \mu(N_+^{(n)}) < \infty$. Since $T_k N_+^{(n)} \subset N_+^{(n)}$, we conclude that $\mu(N_+^{(n)}\backslash T_k N_+^{(n)}) = 0$, so $\mu(N_+^{(n)}\backslash N_-^{(n)}) = 0$. A similar proof shows that $\mu(N_-\backslash N_+) = 0$ so $\mu(N_+ \,\Delta\, N_-) = 0$.

Now suppose $r(t)$ solves Newton's equation and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$. We shall first show that if the energy $E(r(0), \dot{r}(0)) > 0$, then $|r(t)| \geq C|t|$ for t large and use this to prove that $r(t)$ approaches a free solution. Let $I(t) = \frac{1}{2}|r(t)|^2$ be the moment of inertia. Then

$$\dot{I}(t) = \dot{\mathbf{r}} \cdot \mathbf{r} = \dot{r}(t) r(t)$$

where $r(t) = |\mathbf{r}(t)|$ and $\dot{r}(t) = dr/dt$ (which is not equal to $|d\mathbf{r}/dt|$ in general). Also,

$$\begin{aligned} \ddot{I}(t) &= \dot{\mathbf{r}}(t)^2 + \mathbf{F}(\mathbf{r}(t)) \cdot \mathbf{r}(t) \\ &= 2E + \mathbf{r} \cdot \mathbf{F}(\mathbf{r}) - 2V(\mathbf{r}) \end{aligned}$$

Since $E > 0$, and both $r \cdot F$ and V go to zero as $r \to \infty$, we can find R_0 so that $|r| > R_0$ implies $|r \cdot F(r) - 2V(r)| < E$. Since $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, we can find some t_0 with $r(t_0) > R_0$, $\dot{r}(t_0) > 0$. We now claim that $r(t) > R_0$ for all $t > t_0$; for if not, let t_1 be the smallest $t > t_0$ with $r(t) = R_0$. Then $\ddot{I}(t) \geq E$ for $t \in [t_0, t_1]$ so that $\dot{I}(t_1) = r(t_1)\dot{r}(t_1) > \dot{I}(t_0) > 0$. Since $r(t) > R_0$ for $t = t_1 - \varepsilon$ and $r(t_1) = R_0$, we know that $\dot{r}(t_1) \leq 0$, and thus we have a contradiction. It follows that $r(t) > R_0$ for all $t > t_0$ and therefore for all $t > t_0$, $I(t) \geq a + bt + Et^2/2$ for suitable constants a and b. Thus $r(t) \geq \frac{1}{2}t\sqrt{E}$ for t sufficiently large. Using (4), we know that $\int_{t_0}^{\infty} F(r(t))\, dt$ exists, so we can define

$$b = \dot{r}(t_0) + \int_{t_0}^{\infty} F(r(t))\, dt = \lim_{t\to\infty} \dot{r}(t)$$

and

$$a = r(t_0) - bt_0 - \int_{t_0}^{\infty} \int_{s}^{\infty} F(r(t))\, dt\, ds = \lim_{t\to\infty} (r(t) - bt)$$

The second integral also exists. Moreover,

$$\lim_{t\to\infty} |r(t) - a - bt| + |\dot{r}(t) - b| = 0$$

Thus, if $E > 0$ and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, then $r(t)$ is a scattering solution, that is, $\langle r(0), \dot{r}(0)\rangle$ is in Σ_{out}.

Now, let Σ' be Σ with two sets of measure zero removed: namely, $N^+ \,\Delta\, N^-$, which has measure zero by the first part of our proof; and $\{\langle r, v\rangle \mid E(r, v) = 0\}$, which has measure zero since $\{v \mid E(r_0, v) = 0\}$ is a sphere that has measure zero for each fixed $\mathbf{r}_0$. Suppose that $w \in \Sigma' \backslash \Sigma_{\text{bound}}$ and let $r(t)$ be the solution of (2) with $\langle r(0), \dot{r}(0)\rangle = w$. Since $w \notin \Sigma_{\text{bound}}$, either $\overline{\lim}_{t\to-\infty} |r(t)| = \infty$ or $\overline{\lim}_{t\to+\infty} |r(t)| = \infty$ so $w \in (\Sigma \backslash N^+) \cup (\Sigma \backslash N^-)$. Since $w \notin N^+ \,\Delta\, N^- = (\Sigma\backslash N^+) \,\Delta\, (\Sigma \backslash N^-)$, we must have

$w \in (\Sigma \backslash N^+) \cap (\Sigma \backslash N^-)$. By the second part of our argument, since $E(w) \neq 0$, we have $w \in \Sigma_{\text{in}}$ and $w \in \Sigma_{\text{out}}$. This proves that $\Sigma' \backslash \Sigma_{\text{bound}} = \Sigma' \cap \Sigma_{\text{out}} = \Sigma' \cap \Sigma_{\text{in}}$. ∎

Now that we have asymptotic completeness we define the S-transformation.

Definition Let $\Sigma^{(\pm)} = (\Omega^\pm)^{-1}[\Sigma' \backslash \Sigma_{\text{bound}}]$. The ***S*-transformation** is the map $S \colon \Sigma^{(+)} \to \Sigma^{(-)}$ defined by

$$Sw = (\Omega^-)^{-1}(\Omega^+ w)$$

Thus one has the picture shown schematically in Figure XI.1.

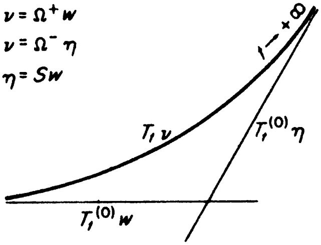


FIGURE XI.1 Schematic picture of scattering.

The S-transformation has thus been defined as a map from $\mathbb{R}^6$ to $\mathbb{R}^6$, or rather from $\mathbb{R}^6$ minus a set of measure 0 to $\mathbb{R}^6$. As a final topic in classical scattering theory, we shall describe a way of "reducing S" to two real-valued functions of two real variables in the case that $\mathbf{F}$ is a **central force**, that is, $V(\mathbf{r})$ is a function of $|\mathbf{r}| = r$ alone. First we note some symmetries of the S-operator. Since $\Omega^\pm T_t^{(0)} = T_t \Omega^\pm$, $ST_t^{(0)} = T_t^{(0)} S$. Since $E(\Omega^\pm w) = E_0(w)$, $E_0(Sw) = E_0(w)$. Finally, rotational invariance of F has two consequences. Let R be an element of $SO(3)$, the family of rotations on three-space. Define R on Σ by $R\langle r, v\rangle = \langle Rr, Rv\rangle$. Then $\Omega^\pm(Rw) = R(\Omega^\pm w)$, so $RS = SR$. Moreover, the angular momentum $\mathbf{L}\langle \mathbf{r}, \mathbf{v}\rangle = \mathbf{v} \times \mathbf{r}$ is conserved, so $\mathbf{L}(Sw) = \mathbf{L}(w)$. We summarize:

Proposition

(a) $ST_t^{(0)} = T_t^{(0)} S$.
(b) $SR = RS$.
(c) $E_0(S\,\cdot) = E_0(\cdot)$.
(d) $\mathbf{L}(S\,\cdot) = \mathbf{L}(\cdot)$.

Conditions (a) and (b) allow us to reduce S to a vector-valued function of only two variables. For the family of sets $\{RT_t^{(0)}w \mid t \in \mathbb{R},\ R \in SO(3)\}$ foliates Σ into a two-parameter family of four-dimensional manifolds (with some exceptional manifolds of smaller dimension), the manifolds of constant E_0 and $|\mathbf{L}|$. By (a) and (b) if we know Sw for one w from each such manifold, we know S for all w. Because of (c) and (d), Sw can lie only on a two-dimensional manifold where E_0 and $\mathbf{L}$ are equal to their values at the point w. Thus we expect S to be parametrized by two real-valued functions of two real variables.

Let us be more explicit: By rotational invariance of S, it is enough to know $S(\mathbf{r}, \mathbf{v})$ when $\mathbf{v} = p\hat{\mathbf{z}}$ and when $\mathbf{r}$ is in the y, z plane, where $\hat{\mathbf{z}}$ is a unit vector in the z direction. If $S\langle \mathbf{r}, \mathbf{v}\rangle = \langle \mathbf{r}', \mathbf{v}'\rangle$, then by property (a), $S\langle \mathbf{r} + \mathbf{v}t, \mathbf{v}\rangle = \langle \mathbf{r}' + \mathbf{v}'t, \mathbf{v}'\rangle$, so we may suppose that $\mathbf{r} \cdot \mathbf{v} = 0$ or $\mathbf{r} = b\hat{\mathbf{y}}$. To summarize, S may be recovered if we know $S\langle b\hat{\mathbf{y}}, p\hat{\mathbf{z}}\rangle$ for all real numbers b and p. Let $S\langle b\hat{\mathbf{y}}, p\hat{\mathbf{z}}\rangle = \langle \mathbf{r}', \mathbf{v}'\rangle$. By conservation of energy $|\mathbf{v}'| = p$ so $\mathbf{v}' = p\hat{\mathbf{e}}(b, p)$ where $\hat{\mathbf{e}}$ is some unit vector. By conservation of angular momentum, $\mathbf{r}'$ and $\mathbf{v}'$ lie in the y, z plane and the component of $\mathbf{r}'$ perpendicular to $\mathbf{v}'$ is determined. There are thus two functions that describe S: **the scattering angle** $\theta = \arccos(\hat{e} \cdot \hat{z})$ and the **time delay** $T = \mathbf{r}' \cdot \hat{e}/p$. These are written as functions of the momentum p and **impact parameter** b, or equivalently as functions of the energy $E = \frac{1}{2}p^2$ and angular momentum $\ell = pb$. One thus has the picture shown in Figure XI.2. Actually, one can explicitly solve the central two-body problem up to quadratures and prove (see Problem 11 or the reference in the Notes):

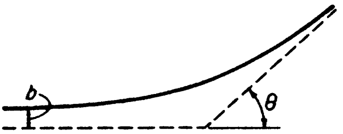


FIGURE XI.2 Central scattering.

$$\theta = \pi - 2\ell \int_{r_0(\ell, E)}^{\infty} [2E - 2V - r^{-2}\ell^2]^{-1/2} \frac{dr}{r^2} \tag{7a}$$

$$\begin{aligned} T = {} & 2 \int_{R_0}^{\infty} \{[2E - r^{-2}\ell^2]^{-1/2} - [2E - 2V - r^{-2}\ell^2]^{-1/2}\}\, dr \\ & -2 \int_{r_0(\ell, E)}^{R_0} [2E - 2V - r^{-2}\ell^2]^{-1/2}\, dr \\ & +2 \int_{\ell/\sqrt{2E}}^{R_0} [2E - r^{-2}\ell^2]^{-1/2}\, dr \end{aligned} \tag{7b}$$

where $r_0(\ell, E) = \sup\{r \mid V(r) + \ell^2/2r^2 > E\}$ and R_0 is any number larger than $\ell/\sqrt{2E}$ and r_0.

Notice that if $V = r^{-1}$ is substituted in (7a) and (7b), the integral for T diverges but the integral for θ converges. This remark will play an important role when we discuss Coulomb scattering in Section 9.

Finally, to make contact with physical experiments, we must define the cross section and its relation to the scattering angle θ. Let us return to the S-transformation in the general situation and consider a slightly different reduction from the one we discussed above. Write $S\langle \mathbf{r}, \mathbf{v}\rangle = \langle \mathbf{f}(\mathbf{r}, \mathbf{v}), \mathbf{g}(\mathbf{r}, \mathbf{v})\rangle$. We shall consider only $\mathbf{g}(\mathbf{r}, v\hat{\mathbf{z}})$. We thus "throw away" the information in f which, in terms of our above analysis, is equivalent to ignoring the time delay. Suppose $v \neq 0$. The relation $ST_t^{(0)} = T_t^{(0)}S$ implies that $\mathbf{g}(\mathbf{r}, v\hat{\mathbf{z}}) = \mathbf{g}(\mathbf{r} + \alpha\hat{\mathbf{z}}, v\hat{\mathbf{z}})$ for any $\alpha \in \mathbb{R}$; thus we consider only $\mathbf{g}(\mathbf{r}, v\hat{\mathbf{z}})$ when $\mathbf{r} \cdot \hat{\mathbf{z}} = 0$. By conservation of energy $|\mathbf{g}| = v$, so $\hat{\mathbf{g}} = \mathbf{g}/v$. We have singled out the function $\hat{\mathbf{g}}(\mathbf{r}, v\hat{\mathbf{z}})$. Fix v. $\hat{g}$ is then a map from $\mathbb{R}^2$, the plane orthogonal to $\hat{z}$ to the unit sphere S^2. Lebesgue measure on $\mathbb{R}^2$ then induces a measure σ on S^2 by

$$\sigma(E) = \mu(\hat{\mathbf{g}}^{-1}(E))$$

where μ is Lebesgue measure on $\mathbb{R}^2$ and E is a Borel subset of S^2. σ is called the **cross-section measure** on S^2. In most cases, σ is absolutely continuous with respect to the usual measure Ω on S^2 when the forward direction $\theta = 0$ is removed. Thus

$$d\sigma = \frac{d\sigma}{d\Omega}\, d\Omega$$

for a function $d\sigma/d\Omega$ on S^2 called the **differential cross section**.

Physical scattering experiments are well described by the following model: A beam of constant energy is sent toward the target. The beam has a wide spread and an approximately uniform density ρ of particles per unit area of the plane $\mathbb{R}^2$ orthogonal to the beam. A detector sits at some scattering angle $\langle\theta, \varphi\rangle$ far from the target and collects (and counts) all particles that leave the target within some angular region of size $\Delta\Omega$ about $\langle\theta, \varphi\rangle$. The measured quantity is

$$\frac{\text{number of particles hitting detector}}{(\Delta\Omega)\rho}$$

The reader should convince herself, that if $\Delta\Omega$ is very small, and the detector and source of particles are very far from the target, this quantity is very close to $d\sigma/d\Omega$. We also note that there is a formula for $(d\sigma/d\Omega)(\theta_0, \varphi_0)$ in the case where $F = -\nabla V$ with $V(r)$ a function of $|\mathbf{r}|$ alone, in terms of the scattering angle θ as a function of E and b, the impact parameter. Explicitly (Problem 12),

$$\left.\frac{d\sigma}{d\Omega}\right|_{\theta=\theta_0} = \sum_{\{b \mid \theta(b)=\theta_0\}} b \csc \theta_0 \left(\frac{d\theta}{db}\right)^{-1} \tag{8}$$

in the case where the sum is finite.

XI.3 The basic principles of scattering in Hilbert space

Quantum dynamics is described by a unitary group on a Hilbert space. Also, as we have seen in Section X.13, the dynamics of classical wave equations can be naturally reformulated in terms of unitary groups. For this reason, the set of basic problems and principles that we present in this section are central to the variety of different scattering theories which we discuss in the remainder of the chapter. We begin with the definition of the generalized wave operators and describe the elementary "kinematics" associated to that notion. The existence of the wave operators is proven in most cases by a general technique known as Cook's method, which we present next. Under suitable conditions that are usually more stringent, one can prove existence *and* completeness by a complex of ideas associated with T. Kato and M. S. Birman. Cook's method and the Kato–Birman theory are the two pillars upon which the abstract time-dependent theory rests. In concrete cases one needs technical tools for showing that the hypotheses of these methods hold—some of these tools are discussed in Appendices 1 and 2 to this section. We end the section with a brief description of some of the ideas in the two Hilbert space theory and the corresponding Kato–Birman-type theorem.

Consider two unitary groups e^{-iAt} and e^{-iBt}, which we think of as an interacting dynamics and a comparison "free" dynamics. What does it mean for $e^{-iAt}\varphi$ to look "asymptotically free" as $t \to -\infty$? Clearly, it means that there is a vector φ_+ such that

$$\lim_{t \to -\infty} \|e^{-iBt}\varphi_+ - e^{-iAt}\varphi\| = 0 \tag{9}$$

Notice that (9) is equivalent to

$$\lim_{t \to -\infty} \|e^{iAt}e^{-iBt}\varphi_+ - \varphi\| = 0$$

so the basic existence question is reduced to the problem of proving the existence of strong limits. In most applications B has purely absolutely continuous spectrum; but in cases where it does not, we need to choose φ_+ in the absolutely continuous subspace for B. For example, if φ_+ were an eigenvector for B, then the strong limit above would exist only if φ_+ is also an eigenvector of A with the same eigenvalue (Problem 15). We therefore define the wave operators by first projecting onto the absolutely continuous subspace of B. When we discuss completeness, it will be clear that this is a very clever choice!

Definition Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ and let $P_{\text{ac}}(B)$ be the projection onto the absolutely continuous subspace of B. We say that the **generalized wave operators** $\Omega^\pm(A, B)$ **exist** if the strong limits

$$\Omega^\pm(A, B) = \operatorname*{s-lim}_{t \to \mp\infty} e^{iAt}e^{-iBt}P_{\text{ac}}(B) \tag{10}$$

exist. When $\Omega^\pm(A, B)$ exist, we define

$$\mathscr{H}_{\text{in}} = \operatorname{Ran} \Omega^+ \qquad \text{and} \qquad \mathscr{H}_{\text{out}} = \operatorname{Ran} \Omega^-$$

For notational convenience, we sometimes use $\mathscr{H}_+$ for $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_-$ for $\mathscr{H}_{\text{out}}$.

The strong limit in (10) turns out to be the right one to take. In case $P_{\text{ac}}(B) = 1$, the *norm* limit exists in (10) only if $A = B$ (Problem 15). On the other hand, as we shall see, if A has purely discrete spectrum, the weak limit in (10) exists (it is 0) even though A and B are very dissimilar.

The funny convention that $t \to \mp\infty$ corresponds to $\Omega^\pm$ is taken from the physics literature and is connected with the relation to the "time-independent theory": As we shall see in Section 6, Ω^+ is related to $\lim_{\varepsilon \downarrow 0} (x + i\varepsilon - A)^{-1}$ and Ω^- to $\lim_{\varepsilon \downarrow 0} (x - i\varepsilon - A)^{-1}$.

The following proposition makes it clear that irrespective of its physical importance, scattering theory is a useful tool in spectral analysis—for this reason parts of this chapter and Chapter XIII are intimately related.

Proposition 1 Suppose that $\Omega^\pm(A, B)$ exist. Then:

(a) $\Omega^\pm$ are partial isometries with initial subspace $P_{\text{ac}}(B)\mathscr{H}$ and final subspaces $\mathscr{H}_\pm$.

(b) $\mathscr{H}_\pm$ are invariant subspaces for A and

$$\Omega^\pm[D(B)] \subset D(A), \qquad A\Omega^\pm(A, B) = \Omega^\pm(A, B)B \tag{11}$$

(c) $\mathscr{H}_\pm \subset \operatorname{Ran} P_{\text{ac}}(A)$.

Proof (a) If $u \in [P_{\mathrm{ac}}(B)\mathscr{H}]^{\perp}$, then clearly $\Omega^{\pm}u = 0$. If $u \in P_{\mathrm{ac}}(B)\mathscr{H}$, then $\|e^{iAt}e^{-iBt}P_{\mathrm{ac}}(B)u\| = \|u\|$ for all t, so $\|\Omega^{\pm}(A, B)u\| = \|u\|$.

(b) Since

$$\operatorname*{s-lim}_{t\to\mp\infty} e^{iAt}e^{-iBt}P_{\mathrm{ac}}(B) = \operatorname*{s-lim}_{t\to\mp\infty} e^{iA(t+s)}e^{-iB(t+s)}P_{\mathrm{ac}}(B)$$

for any fixed s, we have that

$$\Omega^{\pm}(A, B) = e^{iAs}\Omega^{\pm}(A, B)e^{-iBs}$$

or equivalently,

$$e^{-iAs}\Omega^{\pm}(A, B) = \Omega^{\pm}(A, B)e^{-iBs} \tag{12}$$

(11) follows from Stone's theorem and (12). From (12) it is clear that $\mathscr{H}_{\pm}$ are invariant subspaces for e^{-iAs}.

(c) By (a) and (b), $A \restriction \mathscr{H}_{\pm}$ is unitarily equivalent to $B \restriction P_{\mathrm{ac}}(B)\mathscr{H}$ where the unitary equivalence is given by $\Omega^{\pm} : P_{\mathrm{ac}}(B)\mathscr{H} \to \mathscr{H}_{\pm}$. Thus $A \restriction \mathscr{H}_{\pm}$ is purely absolutely continuous. ▮

In quantum theory, where A and B are energy operators, (12) has an interpretation as energy conservation; see Section 4.

The following is often useful:

Proposition 2 (the chain rule) If $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, C)$ exist, then $\Omega^{\pm}(A, C)$ exist and

$$\Omega^{\pm}(A, C) = \Omega^{\pm}(A, B)\Omega^{\pm}(B, C)$$

Proof By Proposition 1c, Ran $\Omega^{\pm}(B, C) \subset$ Ran $P_{\mathrm{ac}}(B)$, so

$$\lim_{t\to\mp\infty} \|(1 - P_{\mathrm{ac}}(B))e^{itB}e^{-itC}P_{\mathrm{ac}}(C)\varphi\| = 0$$

for any φ. Thus,

$$\begin{aligned} e^{itA}e^{-itC}P_{\mathrm{ac}}(C)\varphi &= e^{itA}e^{-itB}P_{\mathrm{ac}}(B)e^{itB}e^{-itC}P_{\mathrm{ac}}(C)\varphi \\ &\quad + e^{itA}e^{-itB}(1 - P_{\mathrm{ac}}(B))e^{itB}e^{-itC}P_{\mathrm{ac}}(C)\varphi \end{aligned}$$

converges to $\Omega^{\pm}(A, B)\,\Omega^{\pm}(B, C)\varphi$ as $t \to \mp\infty$ since a product of strongly convergent families of uniformly bounded operators is strongly convergent. ▮

As discussed in Section 1, weak asymptotic completeness says that $\mathscr{H}_{\mathrm{in}} = \mathscr{H}_{\mathrm{out}}$, while asymptotic completeness says $\mathscr{H}_{\mathrm{in}} = \mathscr{H}_{\mathrm{out}} =$

$[P_{\mathrm{pp}}(A)\mathscr{H}]^{\perp}$ where P_{pp} is the projection onto $\mathscr{H}_{\mathrm{pp}}$, the span of the eigenvectors of A. For the abstract theory, a notion intermediate between these two is appropriate.

Definition Suppose that $\Omega^{\pm}(A, B)$ exist. We say that they are **complete** if and only if

$$\operatorname{Ran} \Omega^{+} = \operatorname{Ran} \Omega^{-} = \operatorname{Ran} P_{\mathrm{ac}}(A)$$

Thus asymptotic completeness is equivalent to the pair of statements: $\Omega^{\pm}$ are complete and $\sigma_{\mathrm{sing}}(A) = \varnothing$. Since the latter statement is purely spectral, it is most naturally studied in a context partially disjoint from scattering theory. We discuss it in Chapter XIII.

The following remarkable fact reduces completeness to an existence question:

Proposition 3 Suppose that $\Omega^{\pm}(A, B)$ exist. Then they are complete if and only if $\Omega^{\pm}(B, A)$ exist.

Proof Suppose that both $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, A)$ exist. Then, by the chain rule, $P_{\mathrm{ac}}(A) = \Omega^{\pm}(A, A) = \Omega^{\pm}(A, B)\Omega^{\pm}(B, A)$, so

$$P_{\mathrm{ac}}(A)\mathscr{H} \subset \operatorname{Ran} \Omega^{\pm}(A, B)$$

Since we already know that $\operatorname{Ran} \Omega^{\pm}(A, B) \subset P_{\mathrm{ac}}(A)\mathscr{H}$, completeness holds.

Conversely, suppose that $\Omega^{\pm}(A, B)$ exist and are complete. Let $\varphi \in P_{\mathrm{ac}}(A)\mathscr{H}$. Then there is a ψ with $\varphi = \Omega^{\pm}(A, B)\psi$. By our discussion at the beginning of the section, this implies that

$$\|e^{-iAt}\varphi - e^{-iBt}P_{\mathrm{ac}}(B)\psi\| \to 0$$

as $t \to -\infty$. Since e^{-iBt} is unitary,

$$\lim_{t \to -\infty} e^{iBt}e^{-iAt}\varphi$$

exists and equals $P_{\mathrm{ac}}(B)\psi$. ∎

At first sight Proposition 3 seems to say that completeness is no harder than existence. In fact, usually completeness is much harder. The reason is that in applications B, which is the comparison free dynamics, is "simple," typically a constant coefficient partial differential operator (or pseudodifferential operator). With the resulting explicit formulas for e^{-iBt} one easily shows that $\Omega^{\pm}(A, B)$ exist by Cook's method. Since one does not have explicit formulas for e^{-iAt}, it is not easy to show $\Omega^{\pm}(B, A)$ exist. Proposition 3 does suggest that one seek some condition on A and B which implies that $\Omega^{\pm}(A, B)$ exist and which is *symmetric* in A and B for then this condition will imply that both $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, A)$ exist, so $\Omega^{\pm}(A, B)$ will exist and be complete. This is the mechanism by which one obtains completeness in the Kato–Birman theory.

* * *

Cook's method is based on the observation that if f is a C^1 function on $\mathbb{R}$ with $f' \in L^1(\mathbb{R})$, then $\lim_{t\to\infty} f(t)$ exists since

$$|f(t) - f(s)| = \left|\int_s^t f'(u)\,du\right| \le \int_s^t |f'(u)|\,du \to 0$$

as $s < t$ both go to ∞.

Theorem XI.4 (Cook's method) Let A and B be self-adjoint operators and suppose that there is a set $\mathscr{D} \subset D(B) \cap P_{\text{ac}}(B)\mathscr{H}$ which is dense in $P_{\text{ac}}(B)\mathscr{H}$ so that for any $\varphi \in \mathscr{D}$ there is a T_0 satisfying:

(a) For $|t| > T_0$, $e^{-iBt}\varphi \in D(A)$;

(b) $\int_{T_0}^{\infty} [\|(B - A)e^{-iBt}\varphi\| + \|(B - A)e^{+iBt}\varphi\|]\,dt < \infty$. (13)

Then $\Omega^{\pm}(A, B)$ exist.

Proof Let $\varphi \in \mathscr{D}$ and let $\eta(t) = e^{iAt}e^{-iBt}\varphi$. Since $e^{-itB}\varphi \in D(A) \cap D(B)$ for $t > T_0$, $\eta(t)$ is strongly differentiable on (T_0, ∞) and

$$\eta'(t) = -ie^{iAt}(B - A)e^{-iBt}\varphi$$

Thus for $t > s > T_0$,

$$\|\eta(t) - \eta(s)\| \le \int_s^t \|\eta'(u)\|\,du \le \int_s^t \|(B - A)e^{-iBu}\varphi\|\,du$$

goes to zero as $s \to \infty$ by (13). Thus $\eta(t)$ is Cauchy as $t \to \infty$, so $\lim_{t\to\infty} e^{iAt}e^{-iBt}P_{\text{ac}}(B)\psi$ exists for all $\psi \in \mathscr{D}$. The limit also exists trivially for all $\psi \in [P_{\text{ac}}(B)\mathscr{H}]^{\perp}$ and, so, by hypothesis for ψ lying in a dense set. Since the family $e^{iAt}e^{-iBt}P_{\text{ac}}(B)$ is a family of uniformly bounded operators, the existence of the limit for a dense set of ψ implies the existence of the limit for all ψ by an $\varepsilon/3$ argument. This proves that Ω^- exists. The proof for Ω^+ is identical. ∎

In applications, one needs to control $\|(B - A)e^{-iBt}\varphi\|$. When B is a constant coefficient differential operator, this can often be done by the method of stationary phase (see Appendix 1).

In some cases one wants a variety of extensions of this theorem. The following is useful when $B - A$ has various "local singularities"; see Section 4:

Theorem XI.5 (Kupsch–Sandhas theorem) Let A and B be self-adjoint operators and suppose that there is a bounded operator χ, and a subspace $\mathscr{D} \subset D(B) \cap P_{\mathrm{ac}}(B)\mathscr{H}$ dense in $P_{\mathrm{ac}}(B)\mathscr{H}$, so that for any $\varphi \in \mathscr{D}$, there is a T_0 satisfying:

(a) for $|t| > T_0$, $(1 - \chi)e^{-iBt}\varphi \in D(A)$;
(b) $\int_{T_0}^{\infty} [\|Ce^{-iBt}\varphi\| + \|Ce^{+iBt}\varphi\|]\, dt < \infty$;

where

$$C = A(1 - \chi) - (1 - \chi)B$$

Suppose, moreover, that for some n, $\chi(B + i)^{-n}$ is compact and that $\mathscr{D} \subset D(B^n)$. Then $\Omega^{\pm}(A, B)$ exist.

This result follows by a simple modification of the proof of Cook's method together with a general result which appears as Lemma 2 below. The reader is asked to provide a proof in Problem 19.

One problem with Cook's method is that it requires $B - A$ to be given to us as an operator rather than a quadratic form. The following result handles the form case:

Theorem XI.6 Let B be a positive self-adjoint operator and let $C_0, \ldots, C_n, D_0, \ldots, D_n$ be closed operators obeying:

(i) $D(C_i) \cap D(D_i) \supset Q(B)$ for $i = 1, \ldots, n$, and

$$\|C_i\varphi\|^2 \le \alpha_i(\varphi, B\varphi) + \beta_i\|\varphi\|^2, \qquad \|D_i\varphi\|^2 \le \alpha_i(\varphi, B\varphi) + \beta_i\|\varphi\|^2$$

for all $\varphi \in Q(B)$.

(ii) $C_0 = 1$, $Q(D_0) \supset Q(B)$, and

$$|(\varphi, D_0\varphi)| \le \alpha_0(\varphi, B\varphi) + \beta_0(\varphi, \varphi)$$

for all $\varphi \in Q(B)$.

(iii) The quadratic form $\sum_{i=0}^{n} C_i^* D_i$ defined on $Q(B)$ is symmetric and $\sum_{i=0}^{n} \alpha_i < 1$.

(iv) There is a set $\mathscr{D}$ contained in $\operatorname{Ran} P_{\mathrm{ac}}(B) \cap D(B)$ which is dense in $P_{\mathrm{ac}}(B)\mathscr{H}$, so that for $\varphi \in \mathscr{D}$,

$$\int_{-\infty}^{\infty} \sum_{i=0}^{n} \|D_i e^{-iBt}\varphi\|\, dt < \infty$$

Then the form sum $A = B + \sum_{i=0}^{n} C_i^* D_i$ is a self-adjoint operator and $\Omega^\pm(A, B)$ exist.

Proof By (i), (ii), and (iii), $\sum_{i=0}^{n} C_i^* D_i$ is a relatively form bounded perturbation of B with relative bound $\alpha \equiv \sum_{i=0}^{n} \alpha_i < 1$. It follows that A is self-adjoint and that $Q(A) = Q(B)$. In particular, the norms

$$\|\varphi\|_B = \|(B+1)^{1/2}\varphi\|, \qquad \|\varphi\|_A = \|(A+E)^{1/2}\varphi\|$$

on $Q(B)$ are equivalent norms, that is,

$$c_1\|\varphi\|_B \le \|\varphi\|_A \le c_2\|\varphi\|_B$$

Here E is some fixed number so that $A + E \ge 1$. e^{-iBt} is clearly an isometry in $\|\cdot\|_B$. Since e^{-iAt} is an isometry in $\|\cdot\|_A$, by the above equivalence, we have that

$$\|e^{-iAt}\varphi\|_B \le c\|\varphi\|_B \tag{14}$$

with $c = c_1^{-1}c_2$ independent of t. Let $W(t) = e^{iAt}e^{-iBt}$. Then for $\varphi \in \mathscr{D}$ and $t \ge s$,

$$\|(W(t) - W(s))\varphi\|^2 = (W(t)\varphi, (W(t) - W(s))\varphi) - (W(s)\varphi, (W(t) - W(s))\varphi)$$

We shall prove that as $t, s \to \infty$, each of these terms goes to zero, so that, as in Cook's theorem, $\Omega^\pm(A, B)$ exist. We consider the first term; the second is similar. We first claim that

$$(W(t)\varphi, (W(t) - W(s))\varphi) = i\int_s^t \sum_{j=0}^{n} (C_j e^{-iAu}W(t)\varphi, D_j e^{-iBu}\varphi)\, du \tag{15}$$

(15) follows (Problem 20) from the hypotheses and the fact that by (14) e^{-iAu} and e^{-iBu} take $Q(B)$ into itself. By (14) and the hypotheses (i), (ii), for all t, u,

$$\sup_j \|C_j e^{-iAu}W(t)\varphi\| \le \gamma\|\varphi\|_B$$

for some γ (*independent of t and u*). It follows by (15) that

$$|(W(t)\varphi, (W(t) - W(s))\varphi)| \le \gamma\|\varphi\|_B \int_s^t \sum_{j=0}^{n} \|D_j e^{-iBu}\varphi\|\, du$$

As in Cook's theorem, by hypothesis (iv), this goes to zero as $s, t \to \infty$. ∎

* * *

We now turn to the complex of results that we designate as the Kato–Birman theory. This theory uses the notion of trace class operator developed in Section VI.6. To describe the idea behind the theory, suppose that $B - A$

is a rank one operator, that is, $(B - A)\varphi = (\psi, \varphi)\psi$. If we tried to use Cook's method to show that $\Omega^{\pm}(A, B)$ exist, we would seek φ with $(\psi, e^{-itB}\varphi) \in L^1(\mathbb{R})$. Since $\varphi \in P_{ac}(B)\mathcal{H}$, we know that the spectral measure $d(\varphi, E_\lambda \varphi)$ equals $|f(\lambda)|^2\, d\lambda$ for some f. We shall see below that it follows that $d(\psi, E_\lambda \varphi) = g(\lambda)|f(\lambda)|^2\, d\lambda$ for some g in $L^2(\mathbb{R}, f^2\, d\lambda)$, and thus

$$(\psi, e^{-itB}\varphi) = \int e^{-it\lambda} g(\lambda)|f(\lambda)|^2\, d\lambda$$

Therefore, $(\psi, e^{-itB}\varphi)$ is the Fourier transform of $(2\pi)^{1/2} g|f|^2$. In general, it is not easy to see when a Fourier transform is in L^1 but to get it to be in L^2 is easy. We therefore begin by finding a set of φ with $(\psi, e^{-itB}\varphi) \in L^2(\mathbb{R})$.

Definition Let B be a self-adjoint operator and $\{E_\Omega\}$ its spectral family. $\mathcal{M}(B)$ will denote the set of all $\varphi \in \mathcal{H}$ such that $d(\varphi, E_\lambda \varphi) = |f(\lambda)|^2\, d\lambda$ where $f \in L^\infty(\mathbb{R})$. We let $|||\varphi|||$ be the L^∞-norm of f.

It is not hard (Problem 17) to prove that $|||\cdot|||$ is a norm and that $\mathcal{M}(B)$ is dense (in the $\mathcal{H}$-norm) in Ran $P_{ac}(B)$.

Lemma 1 For any $\varphi \in \mathcal{M}(B)$ and any $\psi \in \mathcal{H}$,

$$\int |(\psi, e^{-itB}\varphi)|^2\, dt \le 2\pi \|\psi\|^2 |||\varphi|||^2 \tag{16}$$

Proof Let Q be the projection onto the cyclic subspace generated by B and φ. Let $d(\varphi, E_\lambda \varphi) = |f(\lambda)|^2\, d\lambda$. By general spectral theory (see Chapter VII and Section VIII.3) $Q\mathcal{H}$ is unitarily equivalent to $L^2(\mathbb{R}, |f(\lambda)|^2\, d\lambda)$ in such a way that φ corresponds to the vector $\varphi(\lambda) \equiv 1$ and e^{-itB} is multiplication by $e^{-it\lambda}$. Let $\eta(\lambda)$ correspond to the vector $Q\psi$. Then

$$(\psi, e^{-itB}\varphi) = (Q\psi, e^{-itB}\varphi) = \int \eta(\lambda)|f(\lambda)|^2 e^{-it\lambda}\, d\lambda \tag{17}$$

so, by the Plancherel theorem,

$$\begin{aligned}\int |(\psi, e^{-itB}\varphi)|^2\, dt &= 2\pi \int |\eta(\lambda)|^2 |f(\lambda)|^4\, d\lambda \\ &\le 2\pi \|f\|_\infty^2 \int |\eta(\lambda)|^2 |f(\lambda)|^2\, d\lambda\end{aligned}$$

By definition $\|f\|_\infty = |||\varphi|||$ and

$$\int |\eta(\lambda)|^2 |f(\lambda)|^2\, d\lambda = \|Q\psi\|^2 \le \|\psi\|^2 \quad \blacksquare$$

We shall need another simple consequence of thinking of the unitary group in terms of the Fourier transform:

Lemma 2 For any $\varphi \in P_{\mathrm{ac}}(B)$, $e^{-itB}\varphi \to 0$ weakly as $t \to \pm\infty$. If C is compact, then $\|Ce^{-itB}\varphi\| \to 0$ as $t \to \pm\infty$.

Proof By (17) and the fact that f and ηf are in L^2, we have that $(\psi, e^{-itB}\varphi)$ is the Fourier transform of an L^1 function. So, by the Riemann–Lebesgue lemma (Theorem IX.7), $(\psi, e^{-itB}\varphi) \to 0$. Thus, $\|Fe^{-itB}\varphi\| \to 0$ for any finite rank operator F. The result for compact operators follows by an $\varepsilon/3$ argument. ▌

We shall derive the results in the Kato–Birman theory from the following theorem.

Theorem XI.7 (Pearson's theorem) Let A and B be self-adjoint operators and let J be a bounded operator. Suppose that there is a trace class operator C so that $C = AJ - JB$ in the sense that for all $\varphi \in D(A)$ and $\psi \in D(B)$,

$$(\varphi, C\psi) = (A\varphi, J\psi) - (\varphi, JB\psi)$$

then

$$\Omega^{\pm}(A, B; J) \equiv \operatorname*{s-lim}_{t \to \mp\infty} e^{iAt} J e^{-iBt} P_{\mathrm{ac}}(B)$$

exist.

Proof Let $W(t) = e^{iAt} J e^{-iBt}$ and consider the case $t \to \infty$. By the density argument of Cook's method, it suffices to show that

$$\lim_{t < s;\, t \to \infty} \|(W(t) - W(s))\varphi\|^2 = 0 \tag{18}$$

for all $\varphi \in \mathcal{M}(B)$. We shall prove this by writing the left-hand side as two pieces, one to be controlled by Lemma 1 and one by Lemma 2. Let

$$F_{ab}(X) = \int_a^b e^{iBt} X e^{-iBt}\, dt$$

for a bounded operator X and $a < b$. We first claim that

$$W(t)^* W(s) - e^{iaB} W(t)^* W(s) e^{-iaB} = F_{0a}(Y(t, s)) \tag{19}$$

where

$$Y(t, s) = -i[e^{itB}J^*e^{-i(t-s)A}Ce^{-isB} - e^{itB}C^*e^{-i(t-s)A}Je^{-isB}]$$

We shall prove (19) without worrying about domain questions, leaving the reader to take matrix elements and fill in these domain details. The idea will be to write the difference on the left as the integral of its derivative. Let

$$Q(b) = e^{ibB}W(t)^*W(s)e^{-ibB}$$

Then

$$\begin{aligned}\frac{dQ(b)}{db} &= ie^{ibB}[Be^{itB}J^*e^{-i(t-s)A}Je^{-isB} - e^{itB}J^*e^{-i(t-s)A}Je^{-isB}B]e^{-ibB}\\ &= ie^{ibB}[e^{itB}J^*e^{-i(t-s)A}Ce^{-isB} - e^{itB}C^*e^{-i(t-s)A}Je^{-isB}]e^{-ibB}\\ &= -e^{ibB}Y(t, s)e^{-ibB}\end{aligned}$$

Thus (19) follows by integrating the derivative.

For fixed t and s,

$$W(t) - W(s) = i\int_s^t e^{iuA}Ce^{-iuB}\,du$$

is compact, so by Lemma 2,

$$\lim_{a\to\infty} e^{iaB}W(t)^*(W(t) - W(s))e^{-iaB}\varphi = 0$$

for $\varphi \in \mathcal{M}(B)$. It follows by (19) that for $\varphi \in \mathcal{M}(B)$,

$$(\varphi, W(t)^*(W(t) - W(s))\varphi) = \lim_{a\to\infty} (\varphi, F_{0a}(Y(t, t) - Y(t, s))\varphi) \tag{20}$$

Since C is trace class, it has an expansion (see (VI.6)):

$$C = \sum_{n=1}^{\infty} \lambda_n(\varphi_n, \cdot)\psi_n$$

where $\sum \lambda_n = \|C\|_1$, the trace class norm of C, and with $\{\varphi_n\}$ and $\{\psi_n\}$ orthonormal and $\lambda_n > 0$. We claim that for any bounded operator X and $a > 0$,

$$\begin{aligned}&|(\varphi, F_{0a}(e^{iuB}XCe^{-iuB})\varphi)|\\ &\qquad\le (2\pi\|C\|_1)^{1/2}\|X\|\ |||\varphi|||\left[\sum_n \lambda_n \int_u^\infty |(\varphi_n, e^{-ixB}\varphi)|^2\,dx\right]^{1/2}\end{aligned} \tag{21}$$

For, by the canonical expansion above,

$$\begin{aligned}\text{LHS of (21)} &\le \left|\sum_n \lambda_n \int_u^{a+u} (e^{-ixB}\varphi, X\psi_n)(\varphi_n, e^{-ixB}\varphi)\, dx\right| \\ &\le \left[\sum_n \lambda_n \int_{-\infty}^{\infty} |(X\psi_n, e^{-ixB}\varphi)|^2\, dx\right]^{1/2} \\ &\quad \times \left[\sum_n \lambda_n \int_u^{\infty} |(\varphi_n, e^{-ixB}\varphi)|^2\, dx\right]^{1/2} \\ &\le \text{RHS of (21)}\end{aligned}$$

In the second line we used the Schwarz inequality (twice). In the last step, we used Lemma 1. By (20) and (21)

$$\begin{aligned}\|(W(t) - W(s))\varphi\|^2 &\le 8(2\pi\|C\|_1)^{1/2}|||\varphi|||\ \|J\| \\ &\quad \times \left[\sum_n \lambda_n \int_{\min(t,s)}^{\infty} |(\varphi_n, e^{-ixB}\varphi)|^2\, dx\right]^{1/2} \qquad (22)\end{aligned}$$

In the first place, this equation and Lemma 1 imply that

$$\|(W(t) - W(s))\varphi\|^2 \le 16\pi\|C\|_1 |||\varphi|||^2 \|J\| \qquad (23)$$

and, in the second place, since $\sum_n \lambda_n |(\varphi_n, e^{-ixB}\varphi)|^2$ is in L^1, (18) follows. ▌

As a corollary of the theorem and (23), we have:

Corollary Under the hypotheses of Theorem XI.7,

$$\|[\Omega^{\pm}(A, B; J) - J]\varphi\|^2 \le 16\pi\|C\|_1 |||\varphi|||^2 \|J\| \qquad (24)$$

Proof In (23) take $s = 0$ and let $t \to \pm\infty$. ▌

If $AJ - JB$ is trace class, then so is $BJ^* - J^*A$, so both s-lim $e^{iAt}Je^{-iBt}P_{ac}(B)$ and s-lim $e^{iBt}J^*e^{-iAt}P_{ac}(A)$ exist. For general J, this does not imply completeness of either strong limit (for example, consider $J = 0$); but if $J = 1$, Proposition 3 is applicable, so we immediately have the corollary:

Theorem XI.8 (Kato–Rosenblum theorem) If A and B are self-adjoint operators with $A - B \in \mathcal{J}_1$, the trace class, then $\Omega^{\pm}(A, B)$ exist and are complete.

In this theorem A and B may be unbounded. $A - B$ trace class is intended in the sense of Theorem XI.7, that is, $(A\varphi, \psi) = (\varphi, B\psi) + (\varphi, C\psi)$ for some $C \in \mathscr{I}_1$ and $\varphi \in D(A)$, $\psi \in D(B)$. It then follows that $D(A) = D(B)$ and $A\varphi = B\varphi + C\varphi$ for $\varphi \in D(A)$.

Corollary Let $\{A_n\}_{n=1}^{\infty}$, A, B be self-adjoint operators. Suppose that $\Omega^{\pm}(A, B)$ exist and that each $A_n - A$ is trace class with $\|A_n - A\|_1 \to 0$ as $n \to \infty$. Then, for each n, $\Omega^{\pm}(A_n, B)$ exist and

$$\Omega^{\pm}(A, B) = \text{s-lim}\, \Omega^{\pm}(A_n, B)$$

as $n \to \infty$. If $\Omega^{\pm}(B, A)$ exist, then for each n, $\Omega^{\pm}(B, A_n)$ exist and

$$\Omega^{\pm}(B, A)\varphi = \lim_{n\to\infty} \Omega^{\pm}(B, A_n)\varphi$$

for all $\varphi \in \operatorname{Ran} P_{\text{ac}}(A)$.

Proof By the chain rule, it suffices to prove that

$$\operatorname*{s-lim}_{n\to\infty} \Omega^{\pm}(A_n, A) = P_{\text{ac}}(A) \tag{25}$$

and

$$\lim_{n\to\infty} \Omega^{\pm}(A, A_n)\varphi = \varphi \qquad \text{for} \quad \varphi \in \operatorname{Ran} P_{\text{ac}}(A) \tag{26}$$

From the corollary to Theorem XI.7 we immediately conclude that (25) holds. Let φ be in $\operatorname{Ran} P_{\text{ac}}(A)$ and let $\varphi_n = \Omega^{+}(A_n, A)\varphi$. By (25), $\|\varphi_n - \varphi\| \to 0$ as $n \to \infty$. Thus,

$$\|\Omega^{+}(A, A_n)(\varphi_n - \varphi)\| \to 0$$

But, by the completeness of $\Omega^{+}(A_n, A)$, we have that $\Omega^{+}(A, A_n)\varphi_n = \varphi$, so the last limit result says that (26) holds. ∎

It can happen that for $\varphi \in [\operatorname{Ran} P_{\text{ac}}(A)]^{\perp}$, $\Omega^{\pm}(B, A_n)\varphi$ does not go to zero as $n \to \infty$ (Problem 22).

One cannot replace the trace class condition in Theorem XI.8 by a condition that $A - B$ be Hilbert–Schmidt or that $A - B$ be any $\mathscr{I}_p$ with $p > 1$; see the discussion in the Notes. One problem with Theorem XI.8 is that in quantum mechanics $B - A$ is not even bounded.

Theorem XI.9 (Kuroda–Birman theorem) Let A and B be self-adjoint operators so that $(A + i)^{-1} - (B + i)^{-1} \in \mathscr{I}_1$. Then $\Omega^{\pm}(A, B)$ exist and are complete.

Proof Let $J = (A + i)^{-1}(B + i)^{-1}$. Then, in the sense of expectation values,

$$AJ - JB = (B + i)^{-1} - (A + i)^{-1}$$

is trace class, so by Pearson's theorem

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iAt}(A + i)^{-1}(B + i)^{-1}e^{-iBt}P_{\mathrm{ac}}(B)$$

exist. Applying this to a vector of the form $(B + i)\varphi$ with $\varphi \in D(B)$, we conclude that

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iAt}(A + i)^{-1}e^{-iBt}P_{\mathrm{ac}}(B)$$

exist. Now, by hypothesis, $(A + i)^{-1} - (B + i)^{-1}$ is compact, so by Lemma 2,

$$\operatorname*{s-lim}_{t \to \pm\infty}[(A + i)^{-1} - (B + i)^{-1}]e^{-iBt}P_{\mathrm{ac}}(B) = 0$$

It follows that

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iAt}(B + i)^{-1}e^{-iBt}P_{\mathrm{ac}}(B)$$

exist. Applying this to a vector of the form $(B + i)\varphi$, we conclude that $\Omega^{\pm}(A, B)$ exist. It follows by symmetry that $\Omega^{\pm}(B, A)$ exist and thus completeness holds. ▌

To state the next result, we need a technical definition:

Definition Let A and B be self-adjoint operators. We say that A is **subordinate** to B if there are continuous functions f and g on $\mathbb{R}$ with $f(x) \geq 1$, $g(x) \geq 1$, and $\lim_{|x| \to \infty} f(x) = \infty$ such that $D(g(B)) \subset D(f(A))$ and $f(A)g(B)^{-1}$ is bounded. If A is subordinate to B and B is subordinate to A, we say they are **mutually subordinate**.

This condition is very weak. For example, by the closed graph theorem, if $D(A) = D(B)$ or if A and B are semibounded and $Q(A) = Q(B)$, they are mutually subordinate.

Theorem XI.10 (Birman's theorem) Suppose that A and B are self-adjoint operators with spectral projections $E_{\Omega}(A)$, $E_{\Omega}(B)$, respectively. Assume that:

(a) $E_I(A)(A - B)\,E_I(B) \in \mathscr{I}_1$ for every bounded interval I.
(b) A and B are mutually subordinate.

Then $\Omega^{\pm}(A, B)$ exist and are complete.

Proof By symmetry and Proposition 3, it suffices to show that $\Omega^{\pm}(A, B)$ exist. Let $E_a(C) \equiv E_{(-a, a)}(C)$ and $E'_a(C) = E_{(-\infty, -a] \cup [a, \infty)}(C)$ where C is A or B. If $J = E_a(A)E_a(B)$, then $AJ - JB \in \mathscr{I}_1$ by hypothesis (a), so

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{iAt}E_a(A)E_a(B)e^{-iBt}$$

exist by Pearson's theorem. Let $\varphi \in \operatorname{Ran} E_{a_0}(B)$ for some a_0. Then for $a > a_0$ we have that

$$\lim_{t \to \pm\infty} e^{iAt}E_a(A)e^{-iBt}\varphi$$

exist, so to conclude that $\Omega^{\pm}(A, B)\varphi$ exist, it suffices to show that

$$\lim_{a \to \infty} \left[\sup_t \|E'_a(A)e^{-iBt}\varphi\|\right] = 0 \tag{27}$$

Now, let f and g be the functions given by the condition that A is subordinate to B. Let $F(a) = \inf_{|x| \geq a} f(x)$. Then $F(a) \to \infty$ as $a \to \infty$ since $f \to \infty$. Thus:

$$\begin{aligned}\|E'_a(A)e^{-iBt}\varphi\| &\leq F(a)^{-1}\|f(A)E'_a(A)e^{-iBt}\varphi\| \\ &\leq F(a)^{-1}\|f(A)g(B)^{-1}\| \; \|g(B)e^{-iBt}\varphi\| \\ &\leq F(a)^{-1}\|f(A)g(B)^{-1}\| \left[\sup_{|x| \leq a_0} |g(x)|\right] \|\varphi\|\end{aligned}$$

so that (27) holds. ▮

The Kuroda–Birman and Birman theorems have corollaries involving strong convergence similar to the previous corollaries. We leave those to the problems (Problems 23, 24).

There are a large number of conditions that arise in applications but which are not covered by the above considerations. For example, suppose that $A \geq 0$, $B \geq 0$ and $A^2 - B^2 \in \mathscr{I}_1$. Do $\Omega^{\pm}(A, B)$ exist? Or consider $A = -\Delta + V$; $B = -\Delta$ on $\mathbb{R}^n$. For $n \geq 4$, $(A + i)^{-1} - (B + i)^{-1}$ is not trace class for any nontrivial V; but, as we shall see, $(A + E)^{-k} - (B + E)^{-k}$ is trace class so long as k is large enough. Does this imply that $\Omega^{\pm}(A, B)$ exist? The answer to both questions is yes because of the general principle which we are about to describe.

Definition A function φ on T, an open subset of $\mathbb{R}$, is called **admissible** if $T = \bigcup_1^N I_n$ where $I_n = (\alpha_n, \beta_n)$ are disjoint, N is finite or infinite, and:

(a) The distributional derivative φ'' is L^1 on each compact subinterval of T;
(b) on each interval (α_n, β_n), φ' is either *strictly* positive or *strictly* negative.

Example 1 If $T = (0, \infty) = I_1$, then $\varphi(x) = x^{1/2}$ is admissible. Notice that if $A^2 = A_1$, $B^2 = B_1$, then, so long as $A, B \geq 0$, $A = \varphi(A_1)$, $B = \varphi(B_1)$, and $A_1 - B_1 \in \mathscr{I}_1$ if $A^2 - B^2 \in \mathscr{I}_1$.

Example 2 If $T = (0, \infty) = I_1$, then $\varphi(x) = x^{-1/n} - a$ is admissible. Notice that if $A > -a$, $B > -a$, and $A_1 = (A + a)^{-n}$, $B_1 = (B + a)^{-n}$, then $A = \varphi(A_1)$, $B = \varphi(B_1)$, and $A_1 - B_1 \in \mathscr{I}_1$ if $(A + a)^{-n} - (B + a)^{-n} \in \mathscr{I}_1$.

Theorem XI.11 (invariance principle—trace class case) Let φ be an admissible function on an open set T. Suppose that A and B are self-adjoint operators with $\sigma(A), \sigma(B) \subset \bar{T}$ and that at each boundary point of T either φ has a finite limit or both A and B do not have point spectrum at that point. Suppose that $A - B$ is trace class. Then $\Omega^{\pm}(\varphi(A), \varphi(B))$ exist, are complete, and

$$\Omega^{\pm}(\varphi(A), \varphi(B)) = \Omega^{\pm}(A, B)E_{T_1}(B) + \Omega^{\mp}(A, B)E_{T_2}(B)$$

where T_1 (respectively, T_2) is the union of those intervals where $\varphi' > 0$ (respectively, $\varphi' < 0$).

More generally, the same conclusion holds if the condition $A - B \in \mathscr{I}_1$ is replaced by either the hypotheses of Birman's theorem or of the Kuroda–Birman theorem.

The condition at the boundary points is put in only so that $\varphi(A)$ and $\varphi(B)$ can be properly defined.

Before proving this theorem we note that there is a version of it in the case where Cook's method is applicable; see Appendix 3. We also note that on account of Examples 1 and 2 and a continuation of the two examples we have:

Corollary 1 If A and B are positive operators with $A^2 - B^2 \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 2 If A and B are positive operators with $(A^2 + 1)^{-1} - (B^2 + 1)^{-1} \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 3 If A and B are operators with $A, B \geq -a + I$ and $(A + a)^{-k} - (B + a)^{-k} \in \mathscr{I}_1$ for some k, then $\Omega^{\pm}(A, B)$ exist and are complete.

Corollary 4 If A and B are self-adjoint operators and $e^{-A} - e^{-B} \in \mathscr{I}_1$, then $\Omega^{\pm}(A, B)$ exist and are complete.

We return below to conditions which guarantee that the hypotheses of Corollary 3 hold. A weak version of Corollary 3 which is sufficient for all applications can be also proven by the method we used to prove Theorem XI.9 (Problem 25). As preparation for the proof of Theorem XI.11, we need:

Lemma 3 Let φ be an admissible function. Then:

(a) If $Y \subset \mathbb{R}$ has Lebesgue measure zero, then $\varphi[Y \cap T]$ and $\varphi^{-1}[Y]$ have measure zero.

(b) For any $w \in L^2(\alpha_n, \beta_n)$ with $\varphi' > 0$ on (α_n, β_n),

$$\lim_{s \to \infty} \int_0^{\infty} \left| \int_{-\infty}^{\infty} e^{-i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda \right|^2 dt = 0 \tag{28}$$

If $\varphi' < 0$ on (α_n, β_n), $s \to \infty$ should be replaced by $s \to -\infty$ in (28).

Proof (a) See Problem 26.

(b) Since $(2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda$ is the inverse Fourier transform of $e^{is\varphi(\lambda)} w(\lambda)$, the Plancherel theorem implies that

$$2\pi \|w\|^2 \ge \int_0^{\infty} \left| \int_{-\infty}^{\infty} e^{i(t\lambda + s\varphi(\lambda))} w(\lambda)\, d\lambda \right|^2 dt$$

Thus we need prove (28) only for a set of w whose linear combinations are dense in $L^2(\alpha_n, \beta_n)$, say for w the characteristic function of $[a, b] \subset (\alpha_n, \beta_n)$. Since φ'' is L^1 on (α_n, β_n), φ is a C^1 function and thus $\inf_{\lambda \in [a, b]} \varphi'(t) = \gamma > 0$. Using

$$e^{-i(t\lambda + s\varphi(\lambda))} = i(t + s\varphi'(\lambda))^{-1} \frac{d}{d\lambda} (e^{-i(t\lambda + s\varphi(\lambda))})$$

for $t > 0$, $s > 0$, we see that

$$\begin{aligned} &\left| \int_a^b e^{-i(t\lambda + s\varphi(\lambda))}\, d\lambda \right| \\ &\quad = \left| \int_a^b (t + s\varphi'(\lambda))^{-1} \frac{d}{d\lambda} e^{-i(t\lambda + s\varphi(\lambda))}\, d\lambda \right| \\ &\quad \le (t + s\varphi'(b))^{-1} + (t + s\varphi'(a))^{-1} + (t + s\gamma)^{-2} s \int_a^b |\varphi''(\lambda)|\, d\lambda \end{aligned}$$

where we integrate by parts to get to the last inequality. Taking $s \to \infty$ and noting that each term goes to zero in $L^2(0, \infty)$ as a function of t, (28) results. ▌

Proof of Theorem XI.11 Let $C \equiv A - B = \sum \lambda_n(\psi_n, \cdot)\psi_n$ and let

$$\eta \in \operatorname{Ran} E_{(\alpha_n, \beta_n)}(B) \cap \mathcal{M}(B).$$

Then, by (22),

$$\|(\Omega^\pm(A, B) - 1)e^{-i\varphi(B)s}\eta\|^2 \le c\left(\sum_{n=1}^{\infty} |\lambda_n| \int_0^\infty |(\psi_n, e^{-iBt - i\varphi(B)s}\eta)|^2\, dt\right)^{1/2} \tag{29}$$

Now, by Lemma 3b, the individual integrals on the right-hand side of (29) go to zero as $s \to \infty$ (respectively, $s \to -\infty$) if $\varphi' > 0$ ($\varphi' < 0$). Since each integral is bounded on account of Lemma 1 by $2\pi\|\psi_n\|^2|||\eta|||^2$ and $\sum |\lambda_n|\,\|\psi_n\|^2 = \operatorname{Tr}(|C|) < \infty$, the sum on the right-hand side of (29) goes to zero. By Proposition 1, $\Omega^\pm(A, B)e^{-i\varphi(B)s} = e^{-i\varphi(A)s}\Omega^\pm(A, B)$, so

$$\lim_{s \to \pm\infty} e^{i\varphi(A)s}e^{-i\varphi(B)s}\eta = \begin{cases} \Omega^\mp(A, B)\eta & (\varphi' > 0) \\ \Omega^\pm(A, B)\eta & (\varphi' < 0) \end{cases}$$

By Lemma 3a, $P_{\mathrm{ac}}(\varphi(B)) = P_{\mathrm{ac}}(B)$, so the theorem is proven in the case where $A - B$ is trace class.

To prove the theorem under the more general hypotheses, one proceeds as follows: If $AJ - JB$ is in $\mathcal{J}_1$, then

$$\operatorname*{s-lim}_{t \to \pm\infty} e^{i\varphi(A)t}Je^{-i\varphi(B)t}$$

exist and obey a formula analogous to the invariance principle. The proof is identical to the one above. By using this more general result and employing the J's used in the proofs of the Kuroda–Birman and Birman theorems, the invariance principle can be extended to these cases also. The J's are functions of A and B rather than $\varphi(A)$ and $\varphi(B)$. Again, we leave the continuity result to the reader (Problem 28). ▌

Theorem XI.12 Let B be a positive self-adjoint operator and suppose that C is a symmetric form bounded perturbation of B with relative bound $\alpha < 1$ and that

$$(B + 1)^{-\frac{1}{2}}C(B + 1)^{-k-\frac{1}{2}} \in \mathcal{J}_1 \tag{30}$$

Then $A = B + C$ is the form of a self-adjoint operator obeying

$$(A + E)^{-k} - (B + E)^{-k} \in \mathcal{J}_1 \tag{31}$$

for all sufficiently large E. In particular, $\Omega^\pm(A, B)$ exist and are complete.

Proof The last statement follows from (31) and the third corollary of Theorem XI.11. By repeated use of

$$(A+E)^{-1} = (B+E)^{-1} - (A+E)^{-1}C(B+E)^{-1}$$

we find that

$$(A+E)^{-k} = (B+E)^{-k} - \sum_{j=1}^{k}(A+E)^{-j}C(B+E)^{-k+j-1}$$

so that (31) follows from

$$(A+E)^{-j}C(B+E)^{-k-1+j} \in \mathscr{I}_1, \qquad j = 1, \ldots, k \tag{32}$$

By a complex interpolation argument (Problem 29a), this follows from

$$(A+E)^{-\frac{1}{2}}C(B+E)^{-k-\frac{1}{2}} \in \mathscr{I}_1, \qquad (A+E)^{-k-\frac{1}{2}}C(B+E)^{-\frac{1}{2}} \in \mathscr{I}_1 \tag{33}$$

The first part of (33) follows from the hypothesis (30) and the fact that $(A+E)^{-\frac{1}{2}}(B+1)^{\frac{1}{2}}$ is bounded. We need only prove the second part of (33) for E very negative. Choose E so negative that

$$\|(B+E)^{-\frac{1}{2}}C(B+E)^{-\frac{1}{2}}\| = \gamma < 1 \tag{34}$$

Then,

$$(A+E)^{-1} = (B+E)^{-\frac{1}{2}}\left\{\sum_{j=0}^{\infty}[-(B+E)^{-\frac{1}{2}}C(B+E)^{-\frac{1}{2}}]^j\right\}(B+E)^{-\frac{1}{2}}$$

so that

$$\begin{aligned}(B+E)^{-\frac{1}{2}}&(A+E)^{-k}C(B+E)^{-\frac{1}{2}} \\ &= \sum(-1)^{m-1}\left[\prod_{i=1}^{m}(B+E)^{-\frac{1}{2}-\ell_i}C(B+E)^{-\frac{1}{2}}\right]\end{aligned} \tag{35}$$

with the sum over a suitable family of terms with $\ell_1 + \cdots + \ell_m = k$. By a complex interpolation between (30) and (34) (Problem 29b),

$$(B+E)^{-\frac{1}{2}-\ell_i}C(B+E)^{-\frac{1}{2}} \in \mathscr{I}_{k/\ell_i}, \qquad \ell_i = 1, \ldots, k \tag{36}$$

where $\mathscr{I}_p$ is the trace ideal of the appendix to Section IX.4. Using Hölder's inequality for these trace ideals on each term in (35), employing (34) for factors with $\ell_i = 0$ and (36) for terms with $\ell_i > 0$, we see that each term on the right of (35) is in $\mathscr{I}_1$ with a norm bounded by const γ^m. The γ^m makes the sum converge in (35) so that $(B+E)^{-\frac{1}{2}}(A+E)^{-k}C(B+E)^{-\frac{1}{2}}$ is in $\mathscr{I}_1$. Since $(A+E)^{-\frac{1}{2}}(B+E)^{+\frac{1}{2}}$ is bounded, the second part of (33) holds. ▮

The point is that (30) can be verified in a number of applications when B is a differential operator and C is a lower order operator. The main abstract result is described in Appendix 2.

* * *

We close this section with a few words about two Hilbert space scattering theory. In Section 10, we describe physical systems in which the two Hilbert space theory is natural. In that section we give a method for reducing the two Hilbert space problem to a problem on a single space. In typical applications, one can use either that reduction theory or Theorem XI.13 below.

Definition Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, and let J be a bounded operator from $\mathscr{H}_1$ to $\mathscr{H}_2$. We say that $\Omega^{\pm}(A, B; J)$ exist if and only if the strong limits

$$\Omega^{\pm}(A, B; J) = \operatorname*{s-lim}_{t \to \mp\infty} e^{iAt} J e^{-iBt} P_{\text{ac}}(B)$$

exist.

$\Omega^{\pm}(A, B; J)$ may not be isometries. Nevertheless:

Proposition 4 $(\operatorname{Ker} \Omega^+)^{\perp} \equiv \mathscr{H}'_{\text{in}}$ is an invariant space for B and $\mathscr{H}_{\text{in}} = \overline{\operatorname{Ran} \Omega^+}$ is an invariant space for A. Further, $B \restriction \mathscr{H}'_{\text{in}}$ is *unitarily* equivalent to $A \restriction \mathscr{H}_{\text{in}}$. In particular, $A \restriction \mathscr{H}_{\text{in}}$ is purely absolutely continuous.

Proof As in the usual theory,

$$e^{-iAt}\Omega^+ = \Omega^+ e^{-iBt} \tag{37}$$

from which it follows that e^{-iBt} (respectively, e^{-iAt}) leaves $\mathscr{H}'_{\text{in}}$ (respectively, $\mathscr{H}_{\text{in}}$) invariant. The polar decomposition of an operator from $\mathscr{H}_1$ to itself is easily seen to extend to operators from $\mathscr{H}_1$ to $\mathscr{H}_2$. The result is that Ω^+ has a decomposition $\Omega^+ = V|\Omega^+|$ with $|\Omega^+| = [(\Omega^+)^*\Omega^+]^{1/2}$ in $\mathscr{L}(\mathscr{H}_1)$ and V a partial isometry with initial space $\mathscr{H}'_{\text{in}}$ in $\mathscr{H}_1$ and final subspace $\mathscr{H}_{\text{in}} \subset \mathscr{H}_2$. We claim that

$$e^{-iAt}V = Ve^{-iBt} \tag{38}$$

from which the claimed unitary equivalence will follow. By (37), $(\Omega^+)^*e^{-iAt} = e^{-iBt}(\Omega^+)^*$, whence

$$(\Omega^+)^*\Omega^+e^{-iBt} = (\Omega^+)^*e^{-iAt}\Omega^+ = e^{-iBt}(\Omega^+)^*(\Omega^+)$$

By the uniqueness of the positive square root (Theorem VI.9),

$$|\Omega^+|e^{-iBt} = e^{-iBt}|\Omega^+|$$

so (37) implies that

$$e^{-iAt}V|\Omega^+| = Ve^{-iBt}|\Omega^+|$$

As a result, (38) holds applied to vectors in $\overline{\text{Ran }|\Omega^+|}$. To complete the proof of (38), we note that for vectors φ in $(\text{Ran }|\Omega^+|)^\perp = \text{Ker }|\Omega^+| = \text{Ker } V$, one clearly has that $e^{-iAt}V\varphi = 0$. Moreover, $Ve^{-iBt}\varphi = 0$ since we have seen that e^{-iBt} leaves $\text{Ker }|\Omega^+| = (\mathscr{H}'_{\text{in}})^\perp$ invariant. ∎

It is easy to see that the chain rule now says that if $\Omega^\pm(A, B; J_1)$ and $\Omega^\pm(B, C; J_2)$ exist, then so do $\Omega^\pm(A, C; J_1 J_2)$ and they equal $\Omega^\pm(A, B; J_1)\Omega^\pm(B, C; J_2)$.

One phenomenon that can occur is that $\mathscr{H}'_{\text{in}}$ may not be $\text{Ran } P_{\text{ac}}(B)$; for example, take $J = 0$.

Definition If $(\text{Ker }\Omega^\pm)^\perp = \text{Ran } P_{\text{ac}}(B)$, we call $\Omega^\pm$ **semicomplete**. If also $\overline{\text{Ran }\Omega^\pm} = \text{Ran } P_{\text{ac}}(A)$, we call $\Omega^\pm$ **complete**.

In physical situations it can often happen that there is some arbitrariness in the choice of J. It is therefore important to have criteria which guarantee that $\Omega^\pm(A, B; J_1) = \Omega^\pm(A, B; J_2)$.

Definition We say that two operators $J_1, J_2 \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ are **asymptotically *B*-equivalent** if

$$\operatorname*{s-lim}_{t\to\pm\infty}\{(J_1 - J_2)e^{-iBt}P_{\text{ac}}(B)\} = 0$$

In most applications one proves this by showing that $J_1 - J_2$ is compact or that $(J_1 - J_2)(B + i)^{-k}$ is compact for some k (Problem 18).

Definition Let $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ and $J' \in \mathscr{L}(\mathscr{H}_2, \mathscr{H}_1)$. We say that J' is a ***B*-asymptotic left inverse for *J*** (B-left inverse for short) if and only if $J'J$ is asymptotically B-equivalent to I.

The following analogue to Proposition 3 is left to the reader (Problem 30):

Proposition 5 Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Let $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ and suppose that $\Omega^\pm(A, B; J)$ exist.

(a) Let $J_1 \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$. Then J_1 is asymptotically B-equivalent to J if and only if $\Omega^\pm(A, B; J_1)$ exist *and* equal $\Omega^\pm(A, B; J)$.
(b) If J has a B-left inverse, then $\Omega^\pm$ are semicomplete.
(c) Let J' be any B-left inverse. Then $\Omega^\pm(A, B; J)$ are complete if and only if $\Omega^\pm(B, A; J')$ exist *and* J is an A-asymptotic left inverse for J'.
(d) If J^* is a B-left inverse for J, then $\Omega^\pm(A, B; J)$ are partial isometries with initial space Ran $P_{\text{ac}}(B)$.

We note that Pearson's theorem holds without any change in statement *and* proof if one defines $\mathscr{I}_1(\mathscr{H}_1, \mathscr{H}_2)$ as those operators $A \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ with $(A^*A)^{1/2} \in \mathscr{I}_1(\mathscr{H}_1)$.

Theorem XI.13 (Belopol'skii–Birman theorem) Let B and A be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively, with spectral resolutions $E_\Omega(A)$ and $E_\Omega(B)$. Suppose that $J \in \mathscr{L}(\mathscr{H}_1, \mathscr{H}_2)$ satisfies:

(a) J has a two-sided bounded inverse.
(b) For any bounded interval I,

$$E_I(A)(AJ - JB)E_I(B) \in \mathscr{I}_1$$

(c) For any bounded interval I, $(J^*J - 1)E_I(B)$ is compact;

and *either*:

(d_1) $JD(B) = D(A)$;

or

(d_2) $JQ(B) = Q(A)$.

Then $\Omega^\pm(A, B; J)$ exist, are complete, and are partial isometries with initial space Ran $P_{\text{ac}}(B)$ and final space Ran $P_{\text{ac}}(A)$.

Proof Let $J_I = E_I(A)JE_I(B)$ and $J'_I = E_I(B)J^{-1}E_I(A)$. By the generalized Pearson result and (b), the operators $\Omega^\pm(A, B; J_I)$ and $\Omega^\pm(B, A; J_I^*)$ exist. Moreover, we claim that J'_I is asymptotically A-equivalent to J_I^*. For, by (c), $E_I(B)(J^*J - 1)$ is compact, so $E_I(B)(J^* - J^{-1})$ is compact and thus $J_I^* - J'_I$ is compact. By Lemma 2 we have the claimed asymptotic equivalence. Thus $\Omega^\pm(B, A; J'_I)$ exist by (a) of Proposition 5.

By hypothesis (d), we can use the method of Theorem XI.10 to show that

$$\lim_{a \to \infty} \left| \sup_t (\| E_{(-\infty, -a) \cup (a, \infty)}(A) J e^{-iBt} \varphi \|) \right| = 0$$

for $\varphi \in \operatorname{Ran} E_I(B)$, so $\Omega^{\pm}(A, B; J)$ exist. Similarly, $\Omega^{\pm}(B, A; J^{-1})$ exist. It follows by (c) of Proposition 5 that $\Omega^{\pm}(A, B; J)$ is complete. Using hypothesis (c) *again*, we conclude from (d) of Proposition 5 and Lemma 2 that $\Omega^{\pm}(A, B; J)$ are partial isometries from $\operatorname{Ran} P_{ac}(B)$ to $\operatorname{Ran} P_{ac}(A)$. ▌

Appendix 1 to XI.3: Stationary phase methods

In this appendix we present a method for estimating $[e^{-itB}]\varphi(x)$ in the case where B is a differential or pseudo-differential operator. We then illustrate how the estimates can be used by showing that $\Omega^{\pm}(A, B)$ exist when $A - B$ is multiplication by a suitable function. Finally, we discuss how the estimates can be used to handle the second-order wave equations of Sections 10 and 16.

The key to this method is the idea of stationary phase. We shall rewrite $e^{-itB}\varphi(x)$ as $\int u(k)e^{i\omega f(k)}\,dk$ where $\omega \to \infty$ as $t \to \infty$. As $\omega \to \infty$, the rapid oscillations in $e^{i\omega f(k)}$ tend to cancel one another. The cancellation is least effective at points where f varies most slowly, that is, points with $(\nabla f)(k) = 0$. These are called points of **stationary phase**. We first control the integral at points with $\nabla f \neq 0$ and then analyze the points of stationary phase.

Given an open set $\mathcal{O} \subset \mathbb{R}^n$, let $C^{\ell}(\mathcal{O})$ denote the ℓ-times differentiable functions on $\mathcal{O}$ topologized as a Fréchet space by using the seminorms

$$\|f\|_K = \sup_{k \in K} \sum_{|\alpha| \leq \ell} |D^{\alpha} f(k)|$$

K running through all compact subsets of $\mathcal{O}$. We first prove a result that singles out the points of stationary phase in the asymptotics of integrals of the form $\int e^{i\omega f(k)}u(k)\,dk$.

Theorem XI.14 Let K be a compact subset of $\mathbb{R}^n$. Suppose that f is a real-valued function defined on a neighborhood $\mathcal{O}$ of K such that $f \in C^{\ell+1}(\mathcal{O})$ with grad f nonvanishing on all of K. Then, for all $u \in C_0^{\ell}(K^{\text{int}})$,

$$\left| \int e^{i\omega f(k)} u(k)\,dk \right| \leq c(1 + |\omega|)^{-\ell} \|u\|_{\ell,\infty} \tag{39}$$

where

$$\|u\|_{\ell,\infty} = \sum_{|\alpha| \leq \ell} \|D^{\alpha} u\|_{\infty}$$

Moreover, if $M \subset C^{\ell+1}(\mathcal{O})$ is a compact subset of $C^{\ell+1}$ with $(\operatorname{grad} f)(k)$ nonvanishing for all $k \in K$ and $f \in M$, then the constant c in (39) can be chosen uniformly for all $f \in M$.

Proof First fix f. For each $k \in K$, we can find a neighborhood U_k of k, $a_k > 0$, and $j \in \{1, \ldots, n\}$ so that $|\partial f/\partial k_j| \geq a_k$ for all points in U_k. By the compactness of K, we can cover it with finitely many such sets $U_1, \ldots, U_n$. Now find $\varphi_1, \ldots, \varphi_n \in C_0^\infty(\mathcal{O})$ so that $\operatorname{supp} \varphi_i \subset U_i$ and $\sum \varphi_i(y) = 1$ if $y \in K$. By writing

$$e^{i\omega f(k)}u(k) = \sum_j e^{i\omega f(k)}(u\varphi_j)(k)$$

and using $\|\varphi_j u\|_{\ell,\infty} \leq C\|u\|_{\ell,\infty}$, we see that we are reduced to considering the case where $\partial f/\partial k_1 \geq a > 0$ on all of K.

Since $\partial f/\partial k_1 \neq 0$ on K, we can find, by the implicit function theorem, a neighborhood V_k of any $k \in K$ and a $C^{\ell+1}$ function g so that $g(f(k), k_2, \ldots, k_n) = \langle k_1, \ldots, k_n\rangle$ for all $k \in V_k$. By using the partition of unity $\{\varphi_i\}$ as above, we can suppose that one g works on all of K. Let $\langle y_1, \ldots, y_n\rangle = \langle f(k), k_2, \ldots, k_n\rangle$. Then

$$\begin{aligned}\int u(k)e^{i\omega f(k)}\, dk &= \int u(g(y))e^{i\omega y_1}\left[\frac{\partial f}{\partial k_1}(g(y))\right]^{-1} dy \\ &= \int \left[\left(\frac{1}{i\omega}\frac{\partial}{\partial y_1}\right)^{\ell} e^{i\omega y_1}\right](u \circ g)\left(\frac{\partial f}{\partial k_1}\right)^{-1} dy \\ &= \omega^{-\ell}\int e^{i\omega y_1}\left(i\frac{\partial}{\partial y_1}\right)^{\ell}\left[(u \circ g)\left(\frac{\partial f}{\partial k_1}\right)^{-1}\right] dy\end{aligned}$$

Thus,

$$(1 + |\omega|)^{\ell}\left|\int u(k)e^{i\omega f(k)}\, dk\right| \leq D\|(u \circ g)(\partial f/\partial k_1)^{-1}\|_{\ell,\infty}$$

proving (39).

Looking at the above proof, we see that for some neighborhood N of f in $C^{\ell+1}(\mathcal{O})$, we can use the same U_k, etc., and so obtain (39) with a fixed constant c' for all $f \in N$. Covering M with such neighborhoods, we obtain the final uniformity statement. ∎

Corollary Let $P\colon \mathbb{R}^n \to \mathbb{R}$ be C^∞ and let $u \in \mathscr{S}(\mathbb{R}^n)$ be a function so that $\hat{u}$ has compact support. Let $\mathscr{G}$ be an open set containing the compact set $\{\operatorname{grad} P(k) \mid k \in \operatorname{supp} \hat{u}\}$. Let

$$u_t(\mathbf{x}) = (2\pi)^{-n/2}\int \exp[i(\mathbf{x}\cdot\mathbf{k} - tP(\mathbf{k}))]\hat{u}(\mathbf{k})\, d\mathbf{k} \tag{40a}$$

Then, for any m, there is a c depending on m, u, and $\mathscr{G}$ so that

$$|u_t(\mathbf{x})| \le c(1 + |\mathbf{x}| + |t|)^{-m} \tag{40b}$$

for all $\mathbf{x}$, t with $\mathbf{x}/t$ not in $\mathscr{G}$.

Proof Let $f(k) = (|x| + |t|)^{-1}[x \cdot k - tP(k)]$ and $\omega = |x| + |t|$ so that (40) has the form of (39). Since $\nabla_k f = (|x| + |t|)^{-1}[x - t\, \nabla_k P]$, if $x/t \notin \mathscr{G}$, then $\nabla_k f$ is nonvanishing. Moreover, we can take $x/t \to \infty$ in a fixed direction and get limiting functions whose gradients do not vanish either. Thus, the f's lie in a suitable compact subset of C^{m+1} which yields (40b). ▌

(40) has a beautiful and simple interpretation. Think of a classical system with momentum k and Hamiltonian function $P(k)$ independent of x. Such a system has a constant velocity $v = \nabla P(k)$. Thus a classical "packet" $\hat{u}(k)$ has velocities v in $\mathscr{G}$. (40) says that outside of this classically allowed region, the "quantum" wave packet $u_t(x)$ falls off very rapidly. Next we investigate the contribution of isolated points where grad f vanishes:

Theorem XI.15 Let f be a C^∞ real-valued function defined in a neighborhood of 0 in $\mathbb{R}^n$. Suppose that $(\text{grad}\, f)(0) = 0$ and that the matrix $A_{ij} = (\partial^2 f/\partial k_i\, \partial k_j)(0)$ is invertible. Then there is a neighborhood $\mathcal{O}$ of 0 such that for any $s > n/2$ there is a c so that for all $u \in C_0^\infty(\mathcal{O})$ and $\omega \ge 1$,

$$\left| \int u(k) e^{i\omega f(k)}\, dk \right| \le c\omega^{-n/2} \|u\|_{s,\,\infty} \tag{41}$$

Moreover, given such an f_0, there exist neighborhoods $\mathcal{O}_1$ and $\mathcal{O}_2$ of zero with $\bar{\mathcal{O}}_1 \subset \mathcal{O}_2 \subset \mathcal{O}$, and a neighborhood $\mathscr{N}$ of f_0 in the $C^\ell(\mathcal{O}_2)$ topology (for some ℓ) so that (41) holds for all $u \in C_0^\infty(\mathcal{O}_1)$ and $f \in \mathscr{N}$.

Proof First fix an f satisfying the hypotheses of the theorem. We claim that there exists an $\mathcal{O}$ and a C^∞ invertible map $X \colon \mathcal{O} \to \mathcal{O}'$ such that $X(k) = k + O(k^2)$ and such that

$$f(k) = f(0) + \tfrac{1}{2}(X(k), AX(k)) \tag{42}$$

Since $(\text{grad}\, f)(0) = 0$, by Taylor's theorem with remainder, we have

$$f(k) = f(0) + \tfrac{1}{2}(B(k)k, k)$$

where

$$(B(k))_{ij} = 2 \int_0^1 \frac{\partial^2 f}{\partial k_i\, \partial k_j}(sk)(1 - s)\, ds$$

We now seek a C^∞ $n \times n$ matrix-valued function $R(k)$ so that

$$R^*(k)AR(k) = B(k)$$

for if we then take $X(k) = R(k)k$, (42) will hold. Let M be the vector space of $n \times n$ matrices and M_s be the vector space of symmetric $n \times n$ matrices. Consider the function F from $M \times M_s$ to M_s given by

$$F(R, B) = R^*AR - B$$

Thus $(D_R F)|_{R=I,\, B=A}$, the gradient in the R variables, is the map T from M to M_s given by

$$T(C) = C^*A + AC$$

Given $D \in M_s$, $T(\frac{1}{2}A^{-1}D) = D$; so T is surjective since A is nonsingular. Since $F(I, A) = 0$, it follows by the implicit function theorem that for some neighborhood $\mathscr{A}$ of A, there is a C^∞ function $R\colon \mathscr{A} \to M$ so that

$$R^*(B)AR(B) = B, \qquad R(A) = 1$$

Pick $\mathcal{O}$ so that $B(k) \in \mathscr{A}$ for $k \in \mathcal{O}$. Let

$$X(k) = R(B(k))k$$

Then X is C^∞, obeys (42), and, since $B(k) = A + O(k)$, $R(B(k)) = 1 + O(k)$ so that $X(k) = k + O(k^2)$.

Now, letting $y = X(k)$,

$$\begin{aligned}\left|\int u(k)e^{i\omega f(k)}\, dk\right| &= \left|\int u(X^{-1}(y))e^{i\omega(y,\, Ay)/2}\left[\det\left(\frac{\partial X}{\partial k} \circ X^{-1}(y)\right)\right]^{-1} dy\right| \\ &= \left|\int v(y)e^{i\omega(y,\, Ay)/2}\, dy\right|\end{aligned}$$

with $v(y) = u(X^{-1}(y))[\det(\partial X/\partial k \circ X^{-1}(y))]^{-1}$. By the Plancherel theorem,

$$\int v(y)e^{i\omega(y,\, Ay)/2}\, dy = c_1\omega^{-n/2}\int \check{v}(k)e^{-i(k,\, A^{-1}k)/2\omega}\, dk \tag{43}$$

for a suitable A-dependent constant c_1. Thus

$$\begin{aligned}\left|\int u(k)e^{i\omega f(k)}\, dk\right| &\le |c_1|\omega^{-n/2}\|\check{v}\|_1 \\ &\le c_2\omega^{-n/2}\|(1-\Delta)^{n/2}v\|_2 \\ &\le c\omega^{-n/2}\|u\|_{s,\infty}\end{aligned}$$

It remains to prove the uniformity statement at the end of the theorem.

We first claim that for all f near f_0 in the $C^2(\mathcal{O})$ topology, there exists a unique point $k(f)$ near zero with

$$(\text{grad } f)(k(f)) = 0$$

To see this, let $\mathcal{G}: \mathcal{O} \times C^2(\mathcal{O}) \to \mathbb{R}^n$ be the map

$$\mathcal{G}(k, f) = (\text{grad } f)(k)$$

Then $\mathcal{G}(0, f_0) = 0$ and $D_k \mathcal{G}|_{k=0,\, f=f_0}$ is the invertible map A. The claim thus follows from the implicit function theorem. We can therefore conclude that the uniformity statement holds by noting that the size of $\mathcal{O}$ and the constant c in the above proof depend only on finitely many derivatives. ▮

Corollary Let P be a C^∞ function on $\mathbb{R}^n$ and let $u \in \mathcal{S}(\mathbb{R}^n)$ be a function such that $\hat{u}$ has compact support and such that

$$\text{supp } \hat{u} \cap \{k \mid \det[\partial^2 P/\partial k_i \, \partial k_j] = 0\}$$

is empty. Let $u_t(x)$ be given by (40a). Then

$$|u_t(x)| \leq c|t|^{-n/2} \tag{44}$$

for $|t| > 1$ and all x.

Proof Let $\mathcal{J}$ be a bounded neighborhood of supp $\hat{u}$ such that $\det[\partial^2 P/\partial k_i \, \partial k_j] \neq 0$ for $k \in \bar{\mathcal{J}}$. By the corollary to Theorem XI.14, we need only verify (44) for x/t in $\mathcal{G} = \{\text{grad } P(k) \mid k \in \mathcal{J}\}$. For each $p = x/t$ in $\mathcal{G}$,

$$\nabla_k[(|x| + |t|)^{-1}(x \cdot k - tP(k))]$$

vanishes at a finite number of points in $\mathcal{J}$ so that using a partition of unity and Theorem XI.15, (44) holds for $p = x/t$. By the uniformity part of that theorem, the estimate actually holds for a neighborhood of p. By the compactness of $\bar{\mathcal{G}}$, (44) holds for all x and t. ▮

To see how these estimates can be used in scattering theory, consider:

Theorem XI.16 Let P be a C^∞ real-valued function on $\mathbb{R}^n$ such that

$$M \equiv \{k \mid \text{grad } P(k) = 0 \text{ or } \det(\partial^2 P/\partial k_i \, \partial k_j) = 0\}$$

has measure zero. Let V be a real-valued function on $\mathbb{R}^n$ such that

$$(1 + |x|)^{-m} V \in L^2 \tag{45a}$$

We can take $\rho = \frac{1}{2}(1 + \max \rho_\pm)$. (a) is essentially a kind of finite propagation speed for the Klein–Gordon equation. Since the initial data do not have compact support in x, we cannot expect the solution to vanish when $|x|$ is large compared to t, but it does decay rapidly. Notice that for this kind of "finite propagation speed," the speed is actually less than one.

For use in Section 16, we note the following corollary to Theorem XI.17.

Corollary If φ is a regular wave packet for the Klein–Gordon equation (46) with $m \neq 0$, then

$$\int_{\mathbb{R}^n} |\varphi(x, t)| \, dx \leq C(1 + |t|)^{n/2}$$

Proof Break up the x integral into two pieces: $|x| \leq t$ and $|x| \geq t$. By (b), the first integral is bounded by

$$d(1 + |t|)^{-n/2} \int_{|x| \leq t} d^n x \leq c_1 |t|^{n/2}$$

By (a), the second integral goes to zero faster than any power of $|t|$ and in particular is bounded by c_2. Take $C = \max\{c_1, c_2\}$. ∎

Now consider the case $m = 0$. Theorem XI.14 is applicable and immediately yields

$$|\varphi(x, t)| \leq c_{M,\varepsilon}(|x| + |t| + 1)^{-M} \qquad \text{if} \quad |x| \geq (1 + \varepsilon)|t|$$
$$\qquad\qquad\qquad\qquad\qquad\qquad \text{or} \quad |x| \leq (1 - \varepsilon)|t|$$

We emphasize the requirement that $0 \notin \operatorname{supp} u_\pm$ when $m = 0$, for the last estimate will be false in dimension $n = 1$ if $g = \widehat{\varphi_t(\cdot, 0)}$ satisfies $g(0) \neq 0$. In fact, in one dimension, solutions of $\varphi_{tt} = \varphi_{xx}$ with initial data in $\mathcal{S}$ obey

$$\lim_{t \to \infty} \varphi(x, t) = \frac{1}{2} \int_{-\infty}^{\infty} \varphi_t(y, 0) \, dy \tag{47}$$

for any *fixed* x, so that $\varphi(x, t)$ does not go to zero for $|x| \leq (1 - \varepsilon)|t|$. (47) follows from the explicit form of the solution in one dimension:

$$\varphi(x, t) = \frac{1}{2} \int_{x-t}^{x+t} \varphi_t(y, 0) \, dy + \frac{1}{2}[\varphi(x + t, 0) + \varphi(x - t, 0)]$$

This formula also shows that in the case $n = 1$, $\|\varphi\|_\infty$ does not fall off as $|t|^{-n/2}$; in fact the proof of falloff when $m > 0$ fails to extend since $\{M_{ij}\}$ is no longer invertible. However, $\{M_{ij}\}$ is nonsingular in $n - 1$ directions; so we expect, and shall prove, that φ obeys

$$|\varphi(x, t)| \le d|t|^{-(n-1)/2} \tag{48}$$

It is sufficient to prove (48) in any fixed x direction as long as d is independent of x, so we take $x = \langle x_1, 0, \ldots, 0\rangle$, $x_1 > 0$. Thus, we need to control

$$\varphi_\pm(x, t) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{\pm it|k| + ik_1x_1} u_\pm(k)\, d^nk$$

We shall control φ_- for t positive; the other proofs are similar. Choose $\varepsilon > 0$ so that u_- vanishes in the ball of radius 2ε about zero. Pick χ_1 and χ_2 in $C^\infty(\mathbb{R}^n)$ so that $\chi_1 + \chi_2 = 1$ and $\chi_1(k) = 0$ if $k_1 < \varepsilon$ and $\chi_2(k) = 0$ if $k_1 > \frac{3}{2}\varepsilon$. Write

$$\begin{aligned}\varphi_-(x, t) &= (2\pi)^{-n/2} \int_{k_1 > \varepsilon} e^{-it|k| + ik_1x_1} \chi_1(k) u_-(k)\, dk \\ &\quad + (2\pi)^{-n/2} \int_{\substack{k_1 < 3\varepsilon/2 \\ |k| \ge 2\varepsilon}} e^{-it|k| + ik_1x_1} \chi_2(k) u_-(k)\, dk\end{aligned}$$

Since $\nabla_k(-t|k| + k_1x_1)$ vanishes only when $k_1 > 0$, $k_2 = \cdots = k_n = 0$, the second region of integration contains no points of stationary phase, and so the second integral vanishes faster than any power of t. Thus, we need control only the first integral. We do this by introducing a change of variables which separates the direction of the line of stationary phase. Define

$$\begin{aligned}K_1(k) &= k_1 \\ K_j(k) &= \frac{k_j}{\sqrt{k_2^2 + \cdots + k_n^2}} (|k| - k_1)^{1/2}, \qquad j = 2, \ldots, n\end{aligned}$$

Then $k \to K$ is a diffeomorphism on $\mathcal{N} = \{k \mid k_1 > \varepsilon\}$. Since

$$|k| = K_1 + \sum_{j=2}^n K_j(k)^2$$

we have, for suitable g and h,

$$\begin{aligned}&\left| (2\pi)^{-n/2} \int_{\mathcal{N}} e^{-it|k| + ik_1x_1} \chi_1(k) u_-(k)\, d^nk \right| \\ &\quad = \left| (2\pi)^{-n/2} \int_{K[\mathcal{N}]} \exp\left[iK_1(x_1 - t) - it \sum_{j=2}^n K_j^2 \right] g(K)\, d^nK \right| \\ &\quad \le t^{-(n-1)/2} \int_{\mathbb{R}^{n-1}} \left| \exp\left(-(4ti)^{-1} \sum_{j=2}^n y_j^2 \right) \right| |h(x_1 - t, y_2, \ldots, y_n)|\, d^{n-1}y\end{aligned}$$

from which the estimate (48) follows. We summarize:

Theorem XI.18 Let φ be a regular wave packet for the wave equation (46) with $m = 0$. Then:

(a) For any $\varepsilon > 0$ and any N, there is a $c_{N,\varepsilon}$ so that

$$|\varphi(x, t)| \le c_{N,\varepsilon}(1 + |x| + |t|)^{-N}$$

if $|x| < (1 - \varepsilon)|t|$ or $|x| > (1 + \varepsilon)|t|$.

(b) For some d,

$$|\varphi(x, t)| \le d|t|^{-(n-1)/2}$$

for all x and t.

Our definition of regular wave packet when $m = 0$ includes the condition that the Fourier transforms of the initial data vanish near the origin. Actually, this hypothesis is not necessary for part (b). In fact, using either explicit formulas for the solution or further stationary phase analysis (Problem 33), one can prove that the following holds:

Theorem XI.19 Let $\varphi(x, t)$ be a solution of (46) in the case $m = 0$ with initial data in $\mathscr{S}(\mathbb{R}^n)$. Then:

(a) For any N and $\varepsilon > 0$, there is a $c_{N,\varepsilon}$ so that

$$|\varphi(x, t)| \le c_{N,\varepsilon}(1 + |x| + |t|)^{-N}, \qquad |x| \ge (1 + \varepsilon)|t|$$

(b) For any $\varepsilon > 0$, there is a c so that

$$|\varphi(x, t)| \le c_\varepsilon(1 + |t|)^{-(n-1)}, \qquad |x| \le (1 - \varepsilon)|t|$$

(c) There is a d so that

$$|\varphi(x, t)| \le d(1 + |t|)^{-(n-1)/2} \qquad \text{all } x \text{ and } t$$

When n is even, the result in (b) is the best possible. In fact, if $h = \varphi(\cdot, 0) = 0$ and $\ell = \varphi_t(\cdot, 0)$ is in C_0^∞, then, for x fixed, $\varphi(x, t) \sim c_n t^{-(n-1)} \int \ell(y)\, dy$ with $c_n \ne 0$ if n is even. But when n is odd and greater than one. Huygens' principle assures us that the estimate of part (a) also holds in the region $|x| \le (1 - \varepsilon)|t|$ of part (b).

Appendix 2 to XI.3: Trace ideal properties of $f(x)g(-i\nabla)$

To apply the theorems of the Kato–Birman theory, it is often necessary to prove that certain operators of the form $f(x)g(-i\nabla)$ are trace class. Such operators arise in a variety of other situations also, and it is sometimes sufficient to know weaker information about the singular values $\{\mu_m\}$ than $\sum |\mu_m| < \infty$. Recall that $\mathscr{I}_p$ is the set of A in $\mathscr{L}(\mathscr{H})$ such that $\|A\|_p \equiv (\operatorname{tr}(|A|^p))^{1/p} < \infty$. Properties of $\mathscr{I}_p$ and $\|\cdot\|_p$ may be found in Section VI.6 and in the appendix to Section IX.4. The following results are true:

Theorem XI.20 Let $2 \le q < \infty$ and suppose that $f, g \in L^q(\mathbb{R}^n)$. Then $f(x)g(-i\nabla)$ is in $\mathscr{I}_q$ and

$$\|f(x)g(-i\nabla)\|_q \le (2\pi)^{-n/q}\|f\|_q\|g\|_q$$

Recall that $L^2_\delta(\mathbb{R}^n)$ is the set of f such that $\|f\|_\delta = \|(1+x^2)^{\delta/2}f(x)\|_{L_2} < \infty$.

Theorem XI.21 Suppose that f and g are in $L^2_\delta(\mathbb{R}^n)$ for some $\delta > n/2$. Then $f(x)g(-i\nabla)$ is a trace class operator and

$$\|f(x)g(-i\nabla)\|_1 \le c_{\delta,n}\|f\|_\delta\|g\|_\delta$$

There exist necessary and sufficient conditions that $f(x)g(-i\nabla)$ be trace class (see the Notes). In applications, Theorem XI.21 suffices.

Theorem XI.22 Let $2 < q < \infty$ and suppose that $g \in L^q_w(\mathbb{R}^n)$, $f \in L^q(\mathbb{R}^n)$. Then $f(x)g(-i\nabla)$ is a bounded operator with singular values μ_m obeying

$$|\mu_m| \le d_{q,n}\|f\|_q\|g\|_{q,w}\, m^{-1/q}$$

What we mean when we say that $f(x)g(-i\nabla)$ is in $\mathscr{I}_q$ is that there is an A in $\mathscr{I}_q$ so that

$$(\varphi, A\psi) = (\bar{f}\varphi, g(-i\nabla)\psi)$$

for all φ and ψ in $\mathscr{S}(\mathbb{R}^n)$.

We shall give proofs of Theorems XI.20 and XI.21; the reader can find a reference for Theorem XI.22 in the Notes. We note that Theorem XI.20 cannot be extended to any $q < 2$ (see Problem 36). Theorem XI.21 is closely related to the $q \geq 2$ result since $f \in L_\delta^2(\mathbb{R}^n)$ for $\delta > n/2$ implies that $f \in L^1(\mathbb{R}^n)$, and moreover it is not a much stronger hypothesis than $f \in L^1(\mathbb{R}^n)$. Theorem XI.22 is also related to Theorem XI.20 in that $|\mu_m| \leq cm^{-1/q}$ says that $\sum |\mu_m|^q$ is convergent or only barely divergent so that $f(x)g(-i\nabla)$ is almost in $\mathcal{I}_q$. Theorem XI.22 cannot be extended to allow both f and g to lie in L_w^q. For example, the operator $|x|^{-\alpha}|i\nabla|^{-\alpha}$ is not even compact since it commutes with the unitary group of dilations.

Proof of Theorem XI.20 If $q = \infty$, then f and g are in L^∞ so $\|f(x)g(-i\nabla)\|_{\text{op}} \leq \|f\|_\infty \|g\|_\infty$. If $q = 2$, then $f(x)g(-i\nabla)$ is an integral operator with kernel $f(x)(2\pi)^{-n/2}\check{g}(x-y)$ (see Theorem IX.29), so $f(x)g(-i\nabla)$ is Hilbert–Schmidt and $\|f(x)g(-i\nabla)\|_2 \leq (2\pi)^{-n/2}\|f\|_2 \|g\|_2$. The general case now follows by applying the interpolation methods of the appendix to Section IX.4 (Problem 35). ▮

Proof of Theorem XI.21 Write

$$f(x)g(-i\nabla) = AB$$

where

$$A = f(x)(1-\Delta)^{-\delta/2}(1+x^2)^{\delta/2}$$
$$B = (1+x^2)^{-\delta/2}(1-\Delta)^{\delta/2}g(-i\nabla)$$

Then B is Hilbert–Schmidt by Theorem XI.20. Let h be $(2\pi)^{-n/2}$ times the Fourier transform of $(1+k^2)^{-\delta/2}$. Then A is an integral operator with kernel $f(x)h(x-y)(1+y^2)^{\delta/2}$. Since $f \in L_\delta^2$, in order to prove that A is Hilbert–Schmidt, we need only show that

$$\int (1+y^2)^\delta |h(x-y)|^2 \, dy \leq c(1+x^2)^\delta \tag{49}$$

Now, $(1+k^2)^{-\delta/2}$ has an analytic continuation H to $\{z \mid |\text{Im } z| < 1\}$ which obeys $\int |H(k+i\kappa)|^2 \, dk < \infty$, so the Paley–Wiener principle (see Theorem IX.13) assures us that

$$\int e^{2a|x|} |h(x)|^2 \, dx < \infty$$

for all sufficiently small a. In particular,

$$\int (1+x^2)^\delta |h(x)|^2 \, dx < \infty \tag{50}$$

Since $(1+y^2)^\delta \leq 2^\delta(1+|x-y|^2)^\delta(1+x^2)^\delta$, (49) follows from (50). Thus, since A and B are both Hilbert–Schmidt, their product is trace class. ▮

Appendix 3 to XI.3: A general invariance principle for wave operators

In developing the Kato–Birman theory, a striking invariance principle (Theorem XI.11) for the wave operators appeared. One can ask whether this invariance principle holds under more general hypotheses than the condition that $A - B$ be trace class. Our goal in this appendix is to prove a similar result under a hypothesis of the type used in Cook's method.

Theorem XI.23 Let A and B be self-adjoint operators on a Hilbert space $\mathscr{H}$ and φ a function on a finite interval $(a, b) \subset \mathbb{R}$ such that:

(i) The distributional derivative φ'' is in L^1 and $\varphi'(x) \geq \alpha > 0$ for all $x \in (a, b)$.

(ii) Let I be a compact subinterval of (a, b). Let $\mathscr{D}$ be a dense subset of $E_I(B)P_{\text{ac}}(B)\mathscr{H}$ contained in $\mathscr{M}(B)$ such that for any $u \in \mathscr{D}$, the function

$$w(t) = e^{iAt}e^{-iBt}u$$

is strongly differentiable with $\|w'(t)\| \in L^1(\pm 1, \pm\infty) \cap L^2(\pm 1, \pm\infty)$ and $|t|^\alpha \|w'(t)\| \in L^1(\pm 1, \pm\infty)$ for some $\alpha > 0$.

Then, for any $u \in \mathscr{D}$,

$$\lim_{t \to \mp\infty} e^{i\varphi(A)t}e^{-i\varphi(B)t}u$$

exist and equal $\Omega^\pm(A, B)u$.

In particular, suppose that φ is an admissible function on an open set T with $\sigma(A), \sigma(B) \subset \bar{T}$ so that at each boundary point of T either φ has a finite limit or both A and B do not have point spectrum at that point. Then $\Omega^\pm(\varphi(A), \varphi(B))$ exist and

$$\Omega^\pm(\varphi(A), \varphi(B)) = \Omega^\pm(A, B)E_{T_1}(B) + \Omega^\mp(A, B)E_{T_2}(B)$$

where T_1 (respectively, T_2) is the union of those intervals where $\varphi' > 0$ (respectively, $\varphi' < 0$).

To prove this theorem, we need to develop a theory of Fourier transforms of (weakly) measurable $\mathscr{H}$-valued functions in $L^p(\mathbb{R}; \mathscr{H})$ $(p < \infty)$. The easiest way to define this is to let $\mathscr{S}(\mathbb{R}; \mathscr{H})$ denote the space of C^∞ functions from $\mathbb{R}$ to $\mathscr{H}$ with $\sup_\lambda \|(1 + |\lambda|)^n D^\alpha f(\lambda)\| < \infty$ for all α, n. The Fourier transform is then defined as a *weak* integral (recall that all our vector-valued integrals in these volumes are weak integrals),

$$\hat{f}(k) = (2\pi)^{-1/2} \int e^{-ik\lambda} f(\lambda)\, d\lambda \tag{51}$$

By duality, one extends ^ to $\mathscr{S}'(\mathbb{R}; \mathscr{H})$ and thus to $L^p(\mathbb{R}; \mathscr{H}) \subset \mathscr{S}'(\mathbb{R}; \mathscr{H})$. In particular, the Plancherel theorem holds. Indeed, realizing $L^2(\mathbb{R}; \mathscr{H})$ as $L^2(\mathbb{R}) \otimes \mathscr{H}$ as in Section II.4, our extended Fourier transform is just $\mathscr{F} \otimes 1$. Moreover, for $f \in L^1(\mathbb{R}; \mathscr{H})$, (51) holds pointwise.

Let $F \in L^1(\mathbb{R})$. Then, for any $v \in \mathscr{H}$, we claim that

$$\hat{F}(A)v = (2\pi)^{-1/2} \int F(\lambda) e^{-i\lambda A} v\, d\lambda \tag{52}$$

for any self-adjoint A. For (52) holds when $F \in \mathscr{S}(\mathbb{R})$ and so, by a limiting argument it holds for $F \in L^1$.

Fix a function $g \in C_0^\infty(a, b)$ so that $g = 1$ on I and $0 \le g \le 1$. Define

$$G(t, s) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{is\eta - it\varphi(\eta)} g(\eta)\, d\eta$$

Lemma 1 Let φ satisfy hypothesis (i) of Theorem XI.23. Then:

(a) For each fixed t, $G(t, \cdot) \in L^1(\mathbb{R})$.
(b) For each fixed s, $G(t, s) \to 0$ as $t \to \pm\infty$.
(c) $c(t)^2 \equiv \int_{-\infty}^0 |G(t, s)|^2\, ds \to 0$ as $t \to \infty$.
(d) For $v \in \mathscr{H}$ and self-adjoint A,

$$(2\pi)^{-1/2} \int_{-\infty}^{\infty} G(t, s) e^{-isA} v\, ds = e^{-it\varphi(A)} g(A) v$$

Proof (a) For each fixed t, $G(t, \cdot)$ is the Fourier transform of a function of compact support with second derivatives in L^1. Thus $(1 + t^2)G(t, \cdot) \in L^\infty$ so that $G(t, \cdot)$ is certainly in L^1.

(b) Clearly, $|G(t, s)| \le (2\pi)^{-1/2} \|g\|_1$, so it suffices to prove (b) for a g that is a sum of functions of the form $e^{-is\eta} \chi_\Omega(\eta) \varphi'(\eta)$ which are dense in $L^1(I)$. For such g's the result is easy.

(c) is just a restatement of Lemma 3b of Section 3 and (d) follows from (52). ▮

Lemma 2 Let $h \in \mathcal{S}'(\mathbb{R}; \mathcal{H})$ have a Fourier transform in $L^1(\mathbb{R}; \mathcal{H})$ and let C be self-adjoint. Let $G(t, s)$ be as in Lemma 1. Then the integral

$$J_h(t) \equiv \int_{-\infty}^{\infty} G(t, s)e^{-isC}h(s)\, ds$$

exists and

$$\lim_{t \to \pm\infty} \|J_h(t)\| = 0 \tag{53}$$

Proof Since $\hat{h} \in L^1$, h is in L^∞ so the integral exists by Lemma 1a. Let $v \in \mathcal{H}$. Then

$$\begin{aligned}(v, J_h(t)) &= \int_{-\infty}^{\infty} (\overline{G(t, s)}e^{+isC}v, h(s))\, ds \\ &= \int (e^{it\varphi(C-k)}g(C-k)v, \hat{h}(k))\, dk\end{aligned}$$

on account of the Plancherel theorem and Lemma 1d. Thus

$$\|J_h(t)\| \leq \|\hat{h}\|_{L^1} \tag{54}$$

By (54), it suffices to show that (53) holds for a total subset of $\hat{h}$ in L^1, so we consider the case $\hat{h}(k) = f(k)u$; $f \in C_0^\infty(\mathbb{R})$, $u \in \mathcal{H}$. In that case

$$J_h(t) = F_t(C)u$$

where

$$F_t(s) = \int f(k)e^{-it\varphi(s-k)}g(s-k)\, dk$$

Now, $\|F_t\|_\infty \leq \|f\|_1$ for all t, and for each fixed s, $F_t(s) \to 0$ as $t \to \pm\infty$ by Lemma 1b. Thus, by Theorem VII.2d, $\text{s-lim}_{t\to\pm\infty} F_t(C) = 0$, so the lemma is proven. ∎

Lemma 3 Let $h(t)$ be a strongly differentiable function from $\mathbb{R}$ to $\mathcal{H}$ and suppose that:

(i) $\|h(t)\| \to 0$ as $t \to \infty$.
(ii) $\|h'(t)\| \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$.
(iii) $|t|^\alpha \|h'(t)\| \in L^1(\mathbb{R})$ for some $\alpha > 0$.

Then $\hat{h} \in L^1(\mathbb{R}; \mathcal{H})$.

Proof Let G be the Fourier transform of h'. Then by (ii) and (iii), $G \in L^1 \cap L^2$ and

$$\|G(k) - G(\ell)\| \le c_\theta |k - \ell|^\theta$$

for $\theta = \min\{\alpha, 1\}$. By (i),

$$\begin{aligned}\int (v, h'(t))\, dt &= \lim_{a \to \infty} \int_{-a}^{a} (v, h'(t))\, dt \\ &= \lim_{a \to \infty} [(v, h(a)) - (v, h(-a))] = 0\end{aligned}$$

so $G(0) = 0$. It follows that $\|G(k)\| \le c|k|^\theta$. Now let $K(k) = (ik)^{-1}G(k)$. Then $\int_{|k| \ge 1} |K(k)|\, dk < \infty$ since k^{-1} and G are both in $L^2(\pm 1, \pm\infty)$. Moreover, $\int_{-1}^{1} |K(k)|\, dk < \infty$ since $|K(k)| \le C|k|^{\theta - 1}$.

We shall be finished if we prove that $\check{K} = h$. But $\check{K}$ and h have the same derivative, so $\check{K} = h + v$ for some constant vector v. Since $K \in L^1$, $\check{K}(t) \to 0$ as $t \to \infty$ by the Riemann–Lebesgue lemma, so, using hypothesis (i), $v = 0$. ▮

Proof of Theorem XI.23 Fix $u \in \mathscr{D}$ and let

$$I(t) = e^{-it\varphi(A)}\Omega^- u - e^{-it\varphi(B)}u$$

We must show that $I(t) \to 0$ as $t \to \infty$. Let $w(t) = e^{iAt}e^{-iBt}u$ and $w_- = \Omega^- u$. Then, by Lemma 1d and the fact that $g(B)u = u$, and $g(A)\Omega^- u = \Omega^- g(B)u = \Omega^- u$,

$$I(t) = (2\pi)^{-1/2} \int G(t, s)e^{-isA}[w_- - w(s)]\, ds$$

Fix positive C^∞ functions K_0 and $K_\pm$ such that $K_0 \in C_0^\infty$, $\operatorname{supp} K_\pm \subset [\pm 1, \pm\infty)$, and $K_+ + K_- + K_0 = (2\pi)^{-1/2}$. Then $I(t) = \sum_{j=1}^{4} I_j(t)$ where

$$I_j(t) = \int K_{\alpha(j)}(s)G(t, s)e^{-isA}[w_- - w(s)]\, ds$$

for $j = 1, 2$ and $\alpha(1) = 0$, $\alpha(2) = +$,

$$I_3(t) = \int K_-(s)G(t, s)e^{-isA}[w_+ - w(s)]\, ds$$

$$I_4(t) = \int K_-(s)G(t, s)e^{-isA}[w_- - w_+]\, ds$$

with $w_+ = \Omega^+ u$. By the hypotheses, Lemma 2, and Lemma 3, $I_2(t)$ and $I_3(t)$ go to zero as $t \to \infty$. Since

$$|I_1(t)| \le 2\|u\|(2\pi)^{-1/2} \int_{\operatorname{supp} K_0} |G(t, s)|\, ds$$

$I_1(t) \to 0$ as $t \to \infty$ on account of $|G(t, s)| \leq (2\pi)^{-1/2}\|g\|_1$, Lemma 1b and the dominated convergence theorem.

It remains to prove that $I_4(t) \to 0$ as $t \to \infty$. Now, by Lemma 1 in Section 3,

$$\int_{-\infty}^{\infty} |(v, e^{-isB}u)|^2 \, ds \leq 2\pi|||u|||^2\|v\|^2$$

Thus,

$$\begin{aligned}\int_{-\infty}^{\infty} |(v, e^{-isA}w_\pm)|^2 \, ds &\leq \int_{-\infty}^{\infty} |((\Omega^\pm)^*v, e^{-isB}u)|^2 \, ds \\ &\leq 2\pi\|v\|^2|||u|||^2\end{aligned}$$

It follows that

$$\int |K_-(s)|^2 |(v, e^{-isA}(w_- - w_+))|^2 \, ds \leq \text{const}\|v\|^2$$

so that $|I_4(t)| \leq \text{const } c(t)$ where $c(t)$ is given in Lemma 1c. By that lemma, $I_4(t) \to 0$. ▮

In most cases where one really needs the invariance of the wave operators (see Example 1 (revisited) in Section 10 or Example 4 in Section 11), one has already satisfied the hypotheses of the Kato–Birman theory which has the invariance of the wave operators as a corollary. Nevertheless, Theorem XI.23 is interesting since it shows that the invariance principle can hold even when there is no information about asymptotic completeness.

Example 1 Suppose that the hypotheses of Theorem XI.16 hold with (45) replaced by the stronger assumption

$$\int_{+1}^{\infty} t^\alpha \left(\int_{a<|x|<b} |V(xt)|^2 \, dx\right)^{1/2} dt < \infty$$

In particular, this will be true if $|V(x)| \leq c|x|^{-1-\varepsilon}$ near ∞. Then $\Omega^\pm(H^2, H_0^2)$ exist.

Example 2 We want to apply the invariance principle to show the absence of relativistic corrections for electron scattering from external (not necessarily constant) magnetic fields, at least in the approximation that the electron magnetic moment is $e\hbar/mc$ (the physical value differs from this by about 1% due to corrections attributed to quantum electrodynamics). In units with $\hbar = c = 1$, the nonrelativistic Schrödinger Hamiltonian is

$$H_S(A) = \frac{(p - eA)^2}{2m} + \frac{e}{2m}(\sigma \cdot B)$$

acting on $L^2(\mathbb{R}^3; \mathbb{C}^2)$ where, as usual, $p = -i$ grad. Here σ stands for the vector of Pauli spin matrices

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

A is the magnetic vector potential and $B = \operatorname{curl} A$. The relativistic theory is described by the Dirac Hamiltonian

$$H_{\mathrm{D}}(A) = \alpha \cdot (p - eA) + m\beta$$

acting on $L^2(\mathbb{R}^2; \mathbb{C}^4)$. If $\mathbb{C}^4$ is realized as $\mathbb{C}^2 \otimes \mathbb{C}^2$, the conventional choice for α, β is

$$\alpha_i = \sigma_1 \otimes \sigma_i, \qquad \beta = \sigma_3 \otimes 1$$

A direct and elementary formal calculation shows that

$$1 \otimes H_{\mathrm{S}}(A) = (2m)^{-1}[H_{\mathrm{D}}^2(A) - m^2]$$

If A is C^1, with both A and ∇A bounded, then this formal calculation is certainly an equality on the level of self-adjoint operators. If, moreover, $|A(r)| \leq C(1 + r)^{-1-\varepsilon}$, then $\Omega^{\pm}(H_{\mathrm{D}}(A), H_{\mathrm{D}}(0))$ exists by a stationary phase analysis. Moreover, the invariance principle, Theorem XI.23, is applicable, so

$$\Omega^{\pm}(H_{\mathrm{D}}(A), H_{\mathrm{D}}(0)) = 1 \otimes \Omega^{\pm}(H_{\mathrm{S}}(A), H_{\mathrm{S}}(0))$$

This demonstrates the absence of relativistic corrections to scattering at least if the scattering is described in terms of position or momentum variables. Of course, if asymptotic velocities or energies are used, one must remember to use the appropriate kinematics.

XI.4 Quantum scattering I: Two-body case

The scattering theory that we shall study in the most detail is scattering for two-body quantum systems or, what is equivalent, a one-body system in an external potential. This is the most thoroughly studied field in scattering theory, and there is a wide variety of interesting results.

The Hilbert space of a two-particle system is

$$\mathscr{H} = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) = L^2(\mathbb{R}^6)$$

The free Hamiltonian is

$$\tilde{H}_0 = -\frac{1}{2\mu_1}\Delta_1 - \frac{1}{2\mu_2}\Delta_2$$

where $\mathbf{r} \in \mathbb{R}^6$ is written $\mathbf{r} = \langle \mathbf{r}_1, \mathbf{r}_2 \rangle$ with $\mathbf{r}_i \in \mathbb{R}^3$ and Δ_i is the three-dimensional Laplacian associated to $\mathbf{r}_i$. The interacting Hamiltonian is

$$\tilde{H} = \tilde{H}_0 + V(\mathbf{r}_1 - \mathbf{r}_2)$$

where V is a function in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Thus Kato's theorem (Theorem X.16) shows that $\tilde{H}$ is self-adjoint on $C_0^\infty(\mathbb{R}^6)$. We shall later place more severe restrictions on V.

First, we change coordinates to separate the center of mass motion. The new coordinates will be

$$\mathbf{R} = (\mu_1 + \mu_2)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2), \qquad \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$$

Let U be the unitary operator on $L^2(\mathbb{R}^6)$ given by

$$(Uf)(\mathbf{x}, \mathbf{y}) = f((\mu_1 + \mu_2)^{-1}(\mu_1\mathbf{x} + \mu_2\mathbf{y}), \mathbf{x} - \mathbf{y})$$

and let $\mathbf{r}_1$ and $\mathbf{r}_2$ denote the obvious coordinate multiplication operators. Denote $U\mathbf{r}_1U^{-1}$ by $\mathbf{R}$ and $U\mathbf{r}_2U^{-1}$ by $\mathbf{r}_{12}$. Then

$$U\tilde{H}U^{-1} = -\frac{1}{2(\mu_1 + \mu_2)}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{r_{12}} + V(\mathbf{r}_{12})$$

$$U\tilde{H}_0U^{-1} = -\frac{1}{2(\mu_1 + \mu_2)}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{r_{12}}$$

where $m^{-1} = \mu_1^{-1} + \mu_2^{-1}$ (Problem 40). We now write $L^2(\mathbb{R}^6) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$ where now the variables are $\mathbf{R}$ and $\mathbf{r}_{12}$. Then, as operators on $\tilde{D} \equiv C_0^\infty(\mathbb{R}^3) \otimes C_0^\infty(\mathbb{R}^3) \subset C_0^\infty(\mathbb{R}^6)$, $U\tilde{H}_0U^{-1}$ and $U\tilde{H}U^{-1}$ can be decomposed as

$$U\tilde{H}_0U^{-1} = h_0 \otimes I + I \otimes H_0$$

$$U\tilde{H}U^{-1} = h_0 \otimes I + I \otimes H$$

where

$$h_0 = -[2\mu_1 + 2\mu_2]^{-1}\Delta$$

$$H_0 = -(2m)^{-1}\Delta$$

$$H = -(2m)^{-1}\Delta + V(r)$$

Thus, $e^{-itU\tilde{H}_0U^{-1}} = e^{-ith_0} \otimes e^{-itH_0}$ and $e^{-itU\tilde{H}U^{-1}} = e^{-ith_0} \otimes e^{-itH}$. Since these differ only in the second factor, we shall define wave operators $\Omega^{\pm}$ and a scattering operator S for the system $\{e^{-itH}, e^{-itH_0}\}$ on $L^2(\mathbb{R}^3)$. The wave and scattering operators for the original system are then given by $U^{-1}(I \otimes \Omega^{\pm})U$ and $U^{-1}(I \otimes S)U$.

The description we have just given of the coordinate change in terms of a unitary operator is the so-called "active" way of looking at a coordinate transformation. There is a second way of looking at the transformation—the so-called "passive" way. In this interpretation, we think of $-\Delta_1 - \Delta_2$ and $-\frac{1}{2}\Delta_{\mathbf{R}} - 2\Delta_{\mathbf{r}_{12}}$ as the *same* operator (rather than as unitarily equivalent operators) written in terms of a different basic set of coordinates. When there are several coordinate changes, as we shall encounter in Section 6, this second "passive" viewpoint is notationally less cumbersome than the first "active" viewpoint. We shall henceforth adopt this second "passive" viewpoint.

Given our discussion in the preceding section, it is clear that the existence of scattering states is equivalent to the existence of $\Omega^{\pm}(H, H_0)$. Notice that the uniqueness of scattering states is trivial, for if both $\|e^{-iHt}\psi_1 - e^{-itH_0}\varphi\|$ and $\|e^{-iHt}\psi_2 - e^{-itH_0}\varphi\|$ go to zero as $t \to -\infty$, then $\psi_1 - \psi_2 = 0$ by the linearity and uniform boundedness of e^{-iHt}.

The basic existence result is the following:

Theorem XI.24 (the Cook–Hack theorem) Let $V \in L^2(\mathbb{R}^3) + L^r(\mathbb{R}^3)$ for $2 \le r < 3$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $H = H_0 + V$. Then $\Omega^{\pm}(H, H_0)$ exist.

We shall give three different proofs, all based on Cook's method, which illustrate the variety of ways one can estimate $\|Ve^{-itH_0}\varphi\|$.

First proof of Theorem XI.24 This is the most "elementary" proof in that it involves only direct calculations and does not require either interpolation or stationary phase ideas. Fix $\gamma > 0$ and let

$$\varphi_\gamma(x) = \gamma^{3/4} \exp(-\tfrac{1}{2}\gamma x^2)$$

Then, we have that

$$(e^{-itH_0}\varphi_\gamma)(x) = \alpha(t)^{3/4} \exp(-\tfrac{1}{2}[\alpha(t) + i\beta(t)]x^2) \tag{55}$$

where $\beta(t)$ is a suitable real-valued function and

$$\alpha(t) = \gamma(1 + 4t^2\gamma^2)^{-1}$$

To prove (55) one need only note that, up to a constant, $\hat{\varphi}_\gamma$ is $\exp(-\frac{1}{2}p^2/\gamma)$ so that $(e^{-itH_0}\varphi_\gamma)\hat{}$ is $\exp(-\frac{1}{2}p^2/(\gamma(t))$ where $\gamma(t)^{-1} = \gamma^{-1} - 2it$. (55) then follows where the constant can be evaluated by using $\|e^{-itH_0}\varphi_\gamma\|_2 = \|\varphi_\gamma\|_2$.

From (55) one easily sees (Problem 42) that for $k > 0$,

$$\|(1 + |x|)^k e^{-itH_0}\varphi_\gamma\|_\infty \leq c(1 + |t|)^{-\frac{3}{2}+k} \tag{56}$$

It follows that

$$\begin{aligned}\|Ve^{-itH_0}\varphi_\gamma\|_2 &\leq c\|(1 + |x|)^{-k}V\|_2(1 + |t|)^{-\frac{3}{2}+k}\\ &\leq c'(\|V_2\|_2 + \|V_r\|_r)(1 + |t|)^{-\frac{3}{2}+k}\end{aligned}$$

if $V = V_2 + V_r \in L^2 + L^r$ and $r^{-1} = \frac{1}{2} + k/(3 + \varepsilon)^{-1}$ for some $\varepsilon > 0$. This follows from Hölder's inequality and the fact that $(1 + |x|)^{-k} \in L^m$ for all $m > 3k^{-1}$. Since $r < 3$, we can take $k < \frac{1}{2}$, so

$$\int \|Ve^{-itH_0}\varphi_\gamma\|_2\, dt < \infty$$

for any γ. Since linear combinations of translates of the φ_γ are dense (Problem 43), this estimate and Cook's method (Theorem XI.4) imply that $\Omega^\pm(H, H_0)$ exist. ∎

Second proof of Theorem XI.24 By Cook's method we need only show that for any $\varphi \in \mathscr{S}$, $f(t) = \|Ve^{-itH_0}\varphi\|_2$ is in $L^1(1, \infty)$. Recall Theorem IX.30, which says that

$$\|e^{-iH_0t}\varphi\|_p \leq t^{-\frac{3}{2}+3/p}\|\varphi\|_q$$

if $\varphi \in \mathscr{S}$ and $q^{-1} = 1 - p^{-1}$, $2 \leq p \leq \infty$. Write $V = V_2 + V_r$ where $V_2 \in L^2$, $V_r \in L^r$ and let $p^{-1} = \frac{1}{2} - r^{-1}$ so $p > 6$. Then, by Hölder's inequality,

$$\begin{aligned}\|Ve^{-iH_0t}\varphi\|_2 &\leq \|V_2\|_2\|e^{-iH_0t}\varphi\|_\infty + \|V_r\|_r\|e^{-iH_0t}\varphi\|_p\\ &\leq \|V_2\|_2\|\varphi\|_1 t^{-\frac{3}{2}} + \|V_r\|_r\|\varphi\|_q t^{-\frac{3}{2}+3/p}\end{aligned}$$

Since $p > 6$, $\frac{3}{2} - 3p^{-1} > 1$ so $f(t) \in L^1(1, \infty)$ which proves the theorem. ∎

Notice that the condition $r < 3$ was crucial since it implied $p > 6$ and the $t^{-\alpha}$ decay with $\alpha > 1$ which is necessary for $f(t)$ to be in $L^1(1, \infty)$. Which $(1 + |r|)^{-\beta}$ potentials are in $L^2 + L^r$? Precisely those with $\beta > 1$. Again, as in the classical case, simple scattering theory breaks down at the Coulomb force. We shall discuss how to modify quantum scattering theory to handle the Coulomb case in Section 9.

Third proof of Theorem XI.24 By Theorem XI.16, it suffices to prove that (45) holds since we can then use stationary phase estimates. Write

$V = V_2 + V_r$ with $V_2 \in L^2$ and $V_r \in L^r$. By Hölder's inequality,

$$\left(\int_{at<|x|<bt} |V_r(x)|^2\,dx\right)^{\frac{1}{2}} \le \|V_r\|_r \left(\int_{at<|x|<bt} dx\right)^{\frac{1}{2}-1/r}$$
$$= C\|V_r\|_r t^{\frac{3}{2}-3/r}$$

Thus,

$$\int_1^\infty \left(\int_{a<|x|<b} |V_r(xt)|^2\,dx\right)^{\frac{1}{2}} dt \le \int_1^\infty Ct^{-3/r}\|V_r\|_r\,dt < \infty$$

since $r < 3$. Since $|V(x)|^2 \le 2|V_2(x)|^2 + 2|V_r(x)|^2$, (45) holds. ▮

This result can be extended in various directions. If $\mathbb{R}^3$ is replaced by $\mathbb{R}^n$ and $n > 3$, then one can see that the theorem holds if the condition $r < 3$ is replaced by $r < n$; all of the above proofs extend. Of course for general $V \in L^2 + L^r$ it may happen that $H_0 + V$ is not essentially self-adjoint on C_0^∞; the arguments work for *any* self-adjoint extension of $(H_0 + V) \restriction C_0^\infty$. When $V \in L^{n/2} + L^r$ $(n \ge 5)$ or $L^{2+\varepsilon} + L^r$ $(n = 4)$, we know that $H_0 + V$ is self-adjoint on $D(H_0)$ by general principles. For $n = 1$ or 2, only the third proof extends; the result appears in Problem 44. A second direction for extension allows local singularities:

Theorem XI.25 Let V be a measurable function on $\mathbb{R}^3$ so that there is an R, an $\varepsilon > 0$, and a C with

$$|V(\mathbf{r})| \le Cr^{-1-\varepsilon} \qquad \text{if} \quad r > R$$

Let H be an operator with the property that $D_R \equiv C_0^\infty(\mathbb{R}^3\backslash\{\mathbf{r}\,|\,r < R\}) \subset D(H)$, H is self-adjoint, and

$$H\varphi = -\Delta\varphi + V\varphi$$

for $\varphi \in D_R$. Let $H_0 = -\Delta$. Then $\Omega^\pm(H, H_0)$ exist.

Proof Let χ be the operator of multiplication by a function in C_0^∞ that is one on the ball of radius R. Then, as in the proof of the Cook–Hack theorem,

$$\|[H(1-\chi) - (1-\chi)H_0]e^{-itH_0}\varphi\| \in L^1$$

since $H(1-\chi) - (1-\chi)H_0 = V(1-\chi) - \Delta\chi - \nabla\chi \cdot \text{grad}$ and

$$\text{grad}(e^{-itH_0}\varphi) = e^{-itH_0}(\text{grad}\ \varphi).$$

Moreover, $\chi(H_0 + 1)^{-1}$ is Hilbert–Schmidt and so compact. By Problem 18, this implies that $\lim_{t\to\infty} \|\chi e^{-itH_0}\varphi\| = 0$. The result now follows from the Kupsch–Sandhas theorem (Theorem XI.5). ▮

Since one has an explicit formula for $e^{-itH_0}\varphi$, one can prove directly that $\lim_{t\to\infty} \|\chi e^{-itH_0}\varphi\| = 0$ without appealing to the abstract result in Problem 18.

Finally, there are quadratic form results.

Theorem XI.26 Let $V = V_1 + V_2$ be a function on $\mathbb{R}^3$ so that $W_1 \equiv (1 + |x|^2)^{\frac{1}{2}+\varepsilon} V_1$ is in $L^{\frac{3}{2}} + L^\infty$ and V_2 is in $L^{\frac{3}{2}} \cap L^{\frac{3}{2}-\delta}$ for some $\varepsilon > 0$ and $\delta > 0$. Let $H_0 = -\Delta$ and $H = H_0 + V$ as a quadratic form sum. Then $\Omega^\pm(H, H_0)$ exist.

Proof Write $V = C_1 D_1 + C_2 D_2$ with $C_1^* = W_1/|W_1|^{\frac{1}{2}}$,

$$D_1 = |W_1|^{\frac{1}{2}}(1 + |x|^2)^{-\frac{1}{2}-\varepsilon},$$

$C_2^* = V_2/|V_2|^{\frac{1}{2}}$ and $D_2 = |V_2|^{\frac{1}{2}}$. Then by hypothesis, $C_1^* C_1$, $D_1^* D_1$, $C_2^* C_2$, and $D_2^* D_2$ are all H_0-form bounded with relative bound zero, so, by Theorem XI.6, it suffices to prove that for $\varphi \in \mathscr{S}(\mathbb{R}^3)$ we have $\|D_1 e^{-itH_0}\varphi\| \in L^1$ and $\|D_2 e^{-itH_0}\varphi\| \in L^1$. Since $D_2 \in L^{3-2\delta}$, the second expression is in L^1 by the proof of Theorem XI.24. Let $f = (1 + |x|^2)^{-\frac{1}{2}-\varepsilon}$. Then since $D_1(H_0 + 1)^{-1}$ is bounded, it suffices to show that $G(t) \equiv \|(H_0 + 1) f e^{-itH_0}\varphi\|$ is in L^1.

$$\begin{aligned}&(H_0 + 1) f e^{-itH_0}\varphi \\ &\qquad = f e^{-itH_0}[(H_0 + 1)\varphi] - 2(\nabla f) e^{-itH_0}(\text{grad } \varphi) - (\Delta f) e^{-itH_0}\varphi\end{aligned}$$

Since φ, $(H_0 + 1)\varphi$, grad φ are in $\mathscr{S}$ and f, ∇f, $-\Delta f$ are in $L^2 + L^{3-\varepsilon}$, we conclude that $G \in L^1$. ▌

We shall prove in Section XIII.4 that for $V \in L^{3/2} + (L^\infty)_\varepsilon$, $\sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$. Since $\sigma_{\text{ac}} \subset \sigma_{\text{ess}}$, we have

Corollary The operator H of Theorem XI.26 obeys $\sigma_{\text{ac}}(H) = [0, \infty)$.

The methods we have developed work for other cases than the pairs $H = -\Delta + V$, $H_0 = -\Delta$. Consider the case $B_0 = -\Delta + x_1$, $B = -\Delta + V + x_1$, where x_1 is the first component of $\mathbf{x}$. This pair describes scattering in a constant external electric field. As a preliminary, we need:

Lemma Let $B_0 = -\Delta + x_1$. Then

$$e^{-itB_0} = e^{-itx_1} e^{-it^3/3} e^{+it^2 p_1} e^{-itH_0}$$

where $H_0 = -\Delta$.

Proof Consider first the one-dimensional case. Let $f(\alpha) = e^{ip^3\alpha}xe^{-ip^3\alpha}$. Then, as an operator from $\mathscr{S}(\mathbb{R})$ to itself, $f(0) = x$ and $f'(\alpha) = 3p^2$. Thus $f(\alpha) = x + 3p^2\alpha$. It follows that for each α, $f(\alpha)$ is essentially self-adjoint on $\mathscr{S}(R)$, and for any bounded Borel function

$$F(x + 3p^2\alpha) = e^{ip^3\alpha}F(x)e^{-ip^3\alpha}$$

Thus

$$\begin{aligned} e^{-it(p^2+x)} &= e^{ip^3/3}e^{-itx}e^{-ip^3/3} \\ &= e^{-itx}e^{i(p-t)^3/3}e^{-ip^3/3} \\ &= e^{-itx}e^{-it^3/3}e^{it^2p}e^{-itp^2} \end{aligned}$$

where in the second step we used $e^{itx}g(p)e^{-itx} = g(p - t)$. In the n-dimensional case, let $\mathbf{p} = \langle p_1, \mathbf{p}_\perp \rangle$. Then

$$e^{-itB_0} = e^{-it(p_1{}^2 + x_1)}e^{-itp_\perp{}^2}$$

So, by the one-dimensional case, the result holds. ∎

Theorem XI.27 (the Avron–Herbst theorem) Let $\mathbf{x} = \langle x_1, \mathbf{x}_\perp \rangle$. Let V be a function on $\mathbb{R}^n$ obeying:

(i) $\displaystyle\int_{|y-x|\le 1} |V(y)|^2\, dy \le C(1 + |x|^2)^N$

for some N and C and *all* x.

(ii) For some k and ℓ with $2\ell - k > 1$ and some x_0,

$$\left(\int_{|y-x|\le 1} |V(y)|^2\, dy\right)^{\frac{1}{2}} \le C(1 + |x_\perp|)^k/(1 + |x_1|)^\ell$$

for all x with $x_1 < -x_0$.

Let $B_0 = -\Delta + x_1$ and let B be some self-adjoint extension of $(B_0 + V) \restriction \mathscr{S}(\mathbb{R}^n)$. Then $\Omega^\pm(B, B_0)$ exist.

Proof By the lemma, for $\varphi \in \mathscr{S}$,

$$\|Ve^{-itB_0}\varphi\|_2^2 = \int |V(x_1 - t^2, x_\perp)|^2 |(e^{-itH_0}\varphi)(x)|^2\, dx$$

Thus by the stationary phase method we only need that, for any a and b bigger than zero, there is a T_0 with

$$\int_{T_0}^\infty \left(\int_{at\le|x|\le bt} |V(x_1 - t^2, x_\perp)|^2\, d^nx\right)^{\frac{1}{2}} t^{-n/2}\, dt < \infty \tag{57}$$

where we have used hypothesis (i) to control the integral over the remaining x. (57) follows easily from hypothesis (ii). ∎

We emphasize that only x_1 very negative is involved in hypothesis (ii). Physically, this is because B_0 pushes the particle out to negative x_1. As an example, if $B = -\Delta - |x_1|$, then $\Omega^\pm(B, -\Delta - x_1)$ and $\Omega^\pm(B, -\Delta + x_1)$ both exist. Obviously, neither is complete by itself.

* * *

The idea of wave operators and Cook's method for proving their existence is also applicable to a variety of time-dependent quantum-mechanical situations. Thus, consider solutions of a time-dependent Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H(t)\psi(t)$$

where we have in mind $H(t) = -\Delta + V(t)$, and each $V(t)$ is multiplication by a real function. In Section X.12 we discussed the solution of this equation and found, under suitable hypotheses, that there exists a strongly continuous two-parameter family of unitaries $U(t, s)$ obeying

$$U(t, s)U(s, v) = U(t, v), \qquad U(s, s) = 1$$

$$\frac{d}{dt}[U(t, s)\psi] = -iH(t)U(t, s)\psi, \qquad \psi \in D(H_0)$$

See Theorem X.71. A simple case where one is certain that solutions of $U(t, 0)\psi$ should exist which asymptotically look like $e^{-itH_0}\psi$ is when $V(t) = V_1 + \varphi(t)V_2$ where φ has compact support and say $V_1, V_2 \in L^2(\mathbb{R}^3)$; in fact using the existence of the limit of $e^{i(H_0+V_1)t}e^{-iH_0t}$ as $t \to \pm\infty$, it is easy to prove that suitable "time-dependent" wave operators exist in this case. Actually, such wave operators exist under very general circumstances, for example, if

$$V(t) = (\cos\omega_1 t)V_1 + (\cos\omega_2 t)V_2$$

At first sight this may seem surprising, for why should $U(t, 0)\psi$ have a simple limit when $H(t)$ continues to oscillate? The reason is simple: Scattering states spread out as $t \to \pm\infty$, so it does not matter what the potential is doing locally so long as it goes to zero at ∞.

Definition Let $U(t, s)$ be the unitary propagator associated to $H(t) = H_0 + V(t)$ according to Theorems X.70 and X.71. We say that the associated wave operators exist if and only if

$$\Omega^{\pm} \equiv \operatorname*{s-lim}_{t \to \mp\infty} U(t, 0)^* e^{-iH_0 t} \tag{58}$$

exist.

Theorem XI.28 Let $V(t) = V_1(t) + V_2(t)$, where $V_1(t)$ is a strongly differentiable $L^2(\mathbb{R}^3)$-valued function and $V_2(t)$ is a strongly differentiable $L^p(\mathbb{R}^3)$-valued function, $2 \leq p \leq \infty$. Suppose that for some $\varepsilon > 0$ and suitable c,

$$\|V_1(t)\|_2 \leq c|t|^{\frac{1}{2}-\varepsilon}, \qquad |t| \geq 1$$
$$\|V_2(t)\|_p \leq c|t|^{\frac{1}{2}-3p^{-1}-\varepsilon}, \qquad |t| \geq 1$$

Then the limits (58) exist.

Proof Let $\varphi, \psi \in \mathscr{S}(\mathbb{R}^3)$. Then, by Theorem X.71,

$$\begin{aligned}\frac{d}{dt}(\varphi, U(t, 0)^* e^{-iH_0 t}\psi) &= \frac{d}{dt}(U(t, 0)\varphi, e^{-iH_0 t}\psi)\\ &= i(\varphi, U(t, 0)^* V(t) e^{-iH_0 t}\psi)\end{aligned}$$

It follows that for $t > s$,

$$\|U(t, 0)^* e^{-iH_0 t}\psi - U(s, 0)^* e^{-iH_0 s}\psi\| \leq \int_s^t \|V(u)e^{-iH_0 u}\psi\|\, du$$

By the hypotheses and the estimates in the second proof of Theorem XI.24, the last integral is convergent. Following Cook's method, we obtain the existence of the limit (58). ∎

Notice the striking feature of Theorem XI.28 in that it allows $V(t)$ to grow as $t \to \infty$! Using stationary phase ideas (Problem 45), one can show that for $V \in L^2$ *with compact support*, $V(t) = \varphi(t)V$ yields wave operators so long as φ is differentiable and of no more than polynomial growth at infinity.

The intertwining relations $e^{-iHs}\Omega^{\pm} = \Omega^{\pm} e^{-iH_0 s}$ do not, in general, have an analogue in the time-dependent case since $U(t + s, t)$ will not generally have a nice limit as $t \to \infty$. However, there is one special case of particular physical interest where there are still some intertwining relations.

Theorem XI.29 Let $V(t)$ obey the hypotheses of Theorem XI.28. Suppose, moreover, that $V(t+T) = V(t)$ for some fixed T and *all* $t \in \mathbb{R}$. Then

$$U(T, 0)\Omega^{\pm} = \Omega^{\pm} e^{-iH_0 T} \tag{59}$$

and in particular $e^{-iH_0 T}$ commutes with the scattering operator $(\Omega^-)^*\Omega^+$.

Proof Under the hypothesis, $U(t+T, s+T) = U(t, s)$, so that $U(nT, 0) = U(T, 0)^n$. Thus

$$U(nT, 0)^* e^{-iH_0(n+1)T} = U(T, 0)U((n+1)T, 0)^* e^{-iH_0(n+1)T}$$

Taking $n \to \infty$, (59) results. ▮

Reintroducing $\hbar$ and letting $\omega = 2\pi/T$, one finds that Theorem XI.29 asserts that while H_0 may not be conserved by scattering, the energy can be changed only by $n\hbar\omega$ where $n = 0, \pm 1, \ldots$. This is a nonrelativistic justification of Planck's original quantization rule!

Much of the scattering theory we shall develop in this volume can be extended to the time-dependent case; we shall seldom do so explicitly in the text, but will give references in the Notes.

* * *

We now return to the basic quantum-mechanical problem of $\Omega^{\pm}(H, H_0)$ with $H_0 = -\Delta$. Completeness of these operators is easily handled with the Kato–Birman theory if V has sufficiently rapid falloff and sufficient local regularity. We shall later give an example where completeness is destroyed by severe local singularities.

Theorem XI.30 Let V be a measurable function on $\mathbb{R}^n$ so that $|V|$ is $-\Delta$-form bounded with relative bound $\alpha < 1$. Define $H = -\Delta + V$ as a form sum and let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. If $V \in L^1(\mathbb{R}^n)$, then $\Omega^{\pm}(H, H_0)$ exist and are complete.

Proof We shall apply Birman's theorem (Theorem XI.10). Since $Q(H) = Q(H_0)$, the operators are mutually subordinate. Thus it suffices to show that $|V|^{\frac{1}{2}}E_I(H_0)$ and $E_I(H)|V|^{\frac{1}{2}}$ are both Hilbert–Schmidt. This follows if we show that $|V|^{\frac{1}{2}}(H_0 + E)^{-m}$ and $|V|^{\frac{1}{2}}(H + E)^{-m}$ are Hilbert–Schmidt for some m and E. By hypothesis, $|V|^{\frac{1}{2}} \in L^2$, so the first of these is Hilbert–Schmidt by Theorem XI.20 so long as $m > \frac{1}{4}n$. By mimicking the proof of

Theorem XI.12, $|V|^{1/2}(H+E)^{-m}$ is also Hilbert–Schmidt: explicitly by interpolation between $(H_0+E)^{-1/2}V(H_0+E)^{-m-1/2}\in\mathscr{I}_2$ and

$$\gamma\equiv\|(H_0+E)^{-1/2}V(H_0+E)^{-1/2}\|<\infty,$$

we see that $|V|^{1/2}(H_0+E)^{-k-1/2}$ and $(H_0+E)^{-1/2}V(H_0+E)^{-k-1/2}$ lie in $\mathscr{I}_{2m/k}$ for $k=1,2,\ldots,m$. Thus picking E so that $\gamma<1$ and expanding $|V|^{1/2}(H+E)^{-m}$, we get a sum over q and l of terms of the form

$$(|V|^{1/2}(H_0+E)^{-\ell_0-1/2})\left[\prod_{i=1}^{q}(H_0+E)^{-1/2}V(H_0+E)^{-\ell_i-1/2}\right](H_0+E)^{-1/2}\tag{60}$$

with $\sum_{i=0}^{q}\ell_i=m$. Using Hölder's inequality for trace ideals, this term is Hilbert–Schmidt with a norm bounded by $c\gamma^q$, so the sum of the Hilbert–Schmidt norms converges. ∎

This last result is somewhat disappointing in that it requires V to be in L^1, and thus it must have $|x|^{-n-\varepsilon}$ falloff more or less. On the other hand, we have existence so long as V has $|x|^{-1-\varepsilon}$ falloff. We shall later prove completeness under these conditions also but only by using more sophisticated methods; see Section XIII.8, Theorem XIII.33 or Section 17 of this chapter. It turns out that in case V is spherically symmetric, the Kato–Birman theory is applicable even if one has only $|x|^{-1-\varepsilon}$ falloff.

Theorem XI.31 Let $H_0=-\Delta$ on $L^2(\mathbb{R}^3)$ and let $V(x)=V(|x|)$ be a function of $r=|x|$ alone. Suppose that

$$\int_1^\infty|V(r)|\,dr+\int_0^1 r|V(r)|\,dr<\infty\tag{61}$$

Then V is H_0-form bounded with relative bound zero and $\Omega^\pm(H,H_0)$ exist and are complete.

Proof Let us decompose $L^2(\mathbb{R}^3)=\bigoplus_{\ell=0}^{\infty}\bigoplus_{m=-\ell}^{\ell}\mathfrak{h}_{\ell m}$ where $\mathfrak{h}_{\ell m}=\{rf(r)Y_{\ell m}(\theta)\}$. Each $\mathfrak{h}_{\ell m}$ is isomorphic to $L^2(0,\infty;dr)\equiv\mathscr{H}$ under the correspondence $rf(r)Y_{\ell m}\leftrightarrow f(r)$ (see Example 4 of the Appendix to Section X.1). Let $h_{0,\ell}=-(d^2/dr^2)+\ell(\ell+1)r^{-2}$ on $\mathscr{H}$ with boundary condition $f(0)=0$ when $\ell=0$. Let $h_0=h_{0,0}$. Then H_0 is isomorphic to $\bigoplus_{\ell,m}h_{0,\ell}$. Let v be multiplication by V on $\mathscr{H}$. We shall prove that

$$\operatorname{Tr}(|v|^{1/2}(h_0+1)^{-1}|v|^{1/2})<\infty\tag{62}$$

This implies that $\lim_{E\to\infty}\||v|^{1/2}(h_0+E)^{-1}|v|^{1/2}\|=0$ so that $|v|$ is h_0 form bounded with relative bound zero. Since $h_0\le h_{0,\ell}$, we obtain that V is H_0 form bounded with relative bound zero. Let $h_\ell=h_{0,\ell}+v$. Decompose

$$(h_\ell+E)^{-1}-(h_{0,\ell}+E)^{-1}=ABCD$$

where $A = (h_\ell + E)^{-1}(h_0 + 1)^{\frac{1}{2}}$ and $D = (h_0 + 1)^{\frac{1}{2}}(h_{0,\ell} + E)^{-1}$ are bounded and $B = (h_0 + 1)^{-\frac{1}{2}}|v|^{\frac{1}{2}}$ and $C = [v/|v|^{\frac{1}{2}}](h_0 + 1)^{-\frac{1}{2}}$ are Hilbert–Schmidt by (62). It follows, by the Kuroda–Birman theorem that $\Omega^\pm(h_\ell, h_{0,\ell})$ exist and are complete so that $\Omega^\pm(H, H_0)$ exist and are complete.

Thus, we need only prove that (62) holds. We claim that

$$\operatorname{Tr}(|v|^{\frac{1}{2}}(h_0 + 1)^{-1}|v|^{\frac{1}{2}}) = \int_0^\infty |V(r)|[e^{-r}(\sinh r)]\, dr \tag{63}$$

From this, (62) follows by using (61) and the estimates

$$\sinh r \le e^r, \qquad \sinh r \le r \cosh r \le re^r$$

for $r \ge 0$. Now, $(h_0 + 1)^{-1}$ is an integral operator with kernel

$$(h_0 + 1)^{-1}(r, r') = e^{-u} \sinh w \qquad u = \max\{r, r'\}, \quad w = \min\{r, r'\}$$

as can be checked easily (Problem 47). Thus $|v|^{\frac{1}{2}}(h_0 + 1)^{-1}|v|^{\frac{1}{2}}$ has an integral kernel

$$K(r, r') = |v(r)|^{\frac{1}{2}}(h_0 + 1)^{-1}(r, r')|v(r')|^{\frac{1}{2}}$$

so (63) corresponds to the formula

$$\operatorname{Tr}(A) = \int_0^\infty K(r, r)\, dr \tag{64}$$

While (64) is heuristically just a continuum analogue of the fact that $\operatorname{Tr}(a_{ij}) = \sum_i a_{ii}$ for finite matrices, it is *not* a general fact for integral operators; this is obvious since $K(r, r')$ is determined only a.e. and $\{(r, r') \mid r = r'\}$ has measure zero! Nevertheless (64) does hold when the kernel $K(r, r')$ is continuous and the operator is positive semidefinite—we shall prove this as a lemma below. The lemma implies (63) when V is continuous, and a simple approximation argument (Problem 48) concludes the proof of (63) for general V. ▌

Lemma Let μ be a Baire measure on a locally compact Haudorff space X. Let $\mathscr{H} = L^2(X, d\mu)$ and let K be a continuous function on $X \times X$. Suppose that:

(i) For any $\varphi \in \kappa(X)$, the continuous functions of compact support, $\iint \overline{\varphi(x)}\varphi(y)K(x, y)\, d\mu(x)\, d\mu(y) \ge 0$. It follows that $K(x, x) \ge 0$.
(ii) $\int K(x, x)\, d\mu(x) < \infty$.

Then, there is a trace class operator A with integral kernel K. Moreover,

$$\operatorname{Tr}(A) = \int K(x, x)\, d\mu(x) \tag{65}$$

Conversely, if A is a positive trace class operator with a continuous kernel K, then (ii) holds and (65) is true.

Proof Suppose that (i) and (ii) hold. Let f be in $\kappa(X)$ and let $K_f(x, y) = f(x)K(x, y)f(y)$. Then K_f is in $L^2(X \times X, d\mu \otimes d\mu)$ so that there is a Hilbert–Schmidt operator A_f with kernel K_f. Let $\{U_1, \ldots, U_n\} = \mathscr{U}$ be a finite set of disjoint Baire sets of finite μ measure and let $P_{\mathscr{U}}$ be the projection in $\mathscr{H}$ onto the span of the characteristic functions of the U_i. Then

$$\mathrm{Tr}(P_{\mathscr{U}} A_f P_{\mathscr{U}}) = \sum_i \int_{U_i \times U_i} \mu(U_i)^{-1} f(x)K(x, y)f(y)\, d\mu(x)\, d\mu(y) \tag{66}$$

Order the $\mathscr{U}$'s by $\mathscr{U} < \mathscr{U}'$ if $\bigcup U_i \subset \bigcup U_i'$ and each U_i' is either disjoint from all the U_i' or contained in some U_i, that is, if and only if Ran $P_{\mathscr{U}} \subset$ Ran $P_{\mathscr{U}'}$. Under this ordering, the set of $\mathscr{U}$'s is a net and: (a) $P_{\mathscr{U}}$ is monotone increasing in $\mathscr{U}$: (b) s-lim $P_{\mathscr{U}} = 1$; (c) as $\mathscr{U}$ goes to "infinity," the right-hand side of (66) converges to $\int f(x)^2 K(x, x)\, d\mu(x)$. By (i), (a), and (b)

$$\mathrm{Tr}(A_f) = \lim_{\mathscr{U}} \mathrm{Tr}(P_{\mathscr{U}} A_f P_{\mathscr{U}})$$

(both sides may be infinite a priori) and so by (c) and (ii), A_f is trace class and

$$\mathrm{Tr}(A_f) = \int f(x)^2 K(x, x)\, d\mu(x)$$

Now order all f's with $0 \leq f \leq 1$ and $f \in \kappa(X)$ by pointwise inequality. Then, for any $\varphi \in \mathscr{H}$,

$$(\varphi, A_f \varphi) \leq \|\varphi\|^2\, \mathrm{Tr}(A_f) \leq \|\varphi\|^2 \int K(x, x)\, d\mu(x)$$

Moreover, for $\varphi \in \kappa(X)$, $\lim_{f \nearrow 1} (\varphi, A_f \varphi)$ trivially exists. By a density argument, and polarization, w-$\lim_{f \nearrow 1} A_f = A$ exists. Moreover, for any finite rank operator B,

$$|\mathrm{Tr}(AB)| = \lim_{f \nearrow 1} |\mathrm{Tr}(A_f B)| \leq \|B\| \lim_{f \nearrow 1} \mathrm{Tr}(A_f) \leq \|B\| \int K(x, x)\, d\mu(x)$$

Thus A is trace class. Taking φ's in $\kappa(X)$, we find that $K(x, y)$ is the integral kernel for A. Finally, (65) follows by repeating the $P_{\mathscr{U}}$ argument.

The converse statement follows from the $P_{\mathscr{U}}$ argument also. ▌

Example 1 (scattering in a magnetic field) Let $H_0 = -\Delta$ on L^2 and

$$H = \sum (i\, \partial_j - a_j(x))^2 + V(x)$$

where V, a_j, a_j^2 are in $L_\delta^2(\mathbb{R}^n)$ with $\delta > \frac{1}{2}n$. Suppose moreover that $Q(H) =$

$Q(H_0)$ so that $(H+E)^{-\frac{1}{2}}\,\partial_j$ are bounded. Then, for any bounded interval I, the four operators

$$E_I(H)\,\partial_j a_j E_I(H_0), \qquad E_I(H) a_j\,\partial_j E_I(H_0),$$
$$E_I(H) a_j^2 E_I(H_0), \qquad \text{and} \qquad E_I(H) V E_I(H_0)$$

are trace class. The last three are trace class by Theorem XI.21 even without the factor of $E_I(H)$. The first is trace class since $E_I(H)\,\partial_j$ is bounded and $a_j E_I(H_0)$ is trace class. It follows that $E_I(H)(H - H_0)E_I(H_0)$ is trace class so that, since $Q(H) = Q(H_0)$, Birman's theorem is applicable. We conclude that $\Omega^\pm(H, H_0)$ exist and are complete.

Example 2 This is a nonphysical example, but it shows the power of Birman's theorem. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let a be in $L^2_\delta(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ and grad a be in $L^2_\delta(\mathbb{R}^n)$, $\delta > \frac{1}{2}n$, and suppose $a \geq 0$. Define

$$H = H_0 + \Delta a \Delta$$

as a sum of quadratic forms. Since $\Delta a \Delta$ is a fourth-order operator, it is a very singular perturbation of H_0. Clearly $Q(H) = Q(H_0) \cap D(a^{\frac{1}{2}}\Delta) \subset Q(H_0)$. Moreover, $D(H_0) \subset Q(H)$. Thus H and H_0 are mutually subordinate. Writing $H - H_0 = \sum_j (\partial_j) a (\partial_j \Delta) + \partial_j(\partial_j a)\Delta$ and using the fact that $E_I(H)\,\partial_j$ is bounded as in Example 1, we see that

$$E_I(H)(H - H_0)E_I(H_0) \in \mathcal{I}_1$$

so that $\Omega^\pm(H, H_0)$ exist and are complete by Birman's theorem.

Theorem XI.25 asserts that local singularities of V are inessential to the question of existence of $\Omega^\pm(-\Delta + V, -\Delta)$. One can ask whether they are also irrelevant to completeness; to a large extent the answer is yes as we shall now describe.

Definition A self-adjoint operator H is called a **strongly semibounded local perturbation of $H_0 = -\Delta$** if and only if:

(i) $Q(H) \subset Q(H_0)$ and $H_0 \leq c_1(H + c_2)$ for suitable constants c_1 and c_2.
(ii) If $f \in \mathcal{D}_{L^\infty}$, the C^∞ functions with $D^\alpha f \in L^\infty$ for all α, and $\varphi \in D(H)$, then $f\varphi \in D(H)$ and

$$H(f\varphi) = f(H\varphi) - 2\nabla f \cdot \nabla\varphi - \varphi\,\Delta f \tag{67}$$

Notice that, by (i), if φ is in $D(H)$, then $\nabla\varphi$ is in L^2. (ii) says that in some sense $H - H_0$ is a multiplication operator.

Proposition

(a) Let $V = V_1 + V_2$ where $V_1 \geq 0$ and in L^1_{loc} and V_2 is $-\Delta$-form bounded with relative bound $\alpha < 1$. Then $H = -\Delta + V$ defined as a form sum on $Q(H_0) \cap Q(V_1)$ is a strongly semibounded local perturbation of H_0.

(b) Suppose that W also obeys the conditions of (a). Let $\tilde{H} = -\Delta + W$. If $f \in \mathscr{D}_{L\infty}$ has support in $\{x \mid V(x) = W(x)\}$, then for all $\varphi \in D(H)$, we have $f\varphi \in D(\tilde{H})$ and $\tilde{H}(f\varphi) = H(f\varphi)$.

Proof (a) Condition (i) is easy, so we need only check condition (ii). Let $\varphi \in C_0^\infty$ and $f \in \mathscr{D}_{L\infty}$. Then clearly $f\varphi \in Q(-\Delta)$ and

$$\nabla(f\varphi) = f\,\nabla\varphi + \varphi\,\nabla f$$

By an easy limiting argument, it follows that if $\varphi \in Q(-\Delta)$, then $f\varphi \in Q(-\Delta)$. Let $\varphi \in Q(-\Delta)$ and $\psi \in C_0^\infty$. Then

$$(\varphi, (-\Delta)f\psi) = (f\varphi, (-\Delta)\psi) - 2((\nabla f)\varphi, \nabla\psi) - ((\Delta f)\varphi, \psi)$$

Again, using a limiting argument, this extends to all $\psi \in Q(H_0)$. Clearly, if $\int V_1 |\varphi|^2\,dx < \infty$, we have that $\int V_1 |f|^2 |\varphi|^2\,dx < \infty$; so if $\psi, \varphi \in Q(H)$, then $f\varphi \in Q(H)$ and

$$(\psi, H(f\varphi)) = (f\psi, H\varphi) - 2((\nabla f)(\psi, \nabla\varphi) - ((\nabla f)\psi, \varphi) \qquad (68)$$

Recall that by the form construction (Section VIII.6) the domain of H consists of those φ in $Q(H)$ such that there is an $\eta \in \mathscr{H}$ satisfying $(\psi, \eta) = (\psi, H\varphi)$ for all ψ in $Q(H)$. In this case $\eta = H\varphi$. Given this and (68), we conclude that if $\varphi \in D(H)$, then $f\varphi$ is in $D(H)$ and (67) holds.

(b) Since $\varphi \in D(H) \subset Q(H)$, $\varphi \in Q(H_0)$ and $\int |\varphi|^2 V_1\,dx < \infty$. Since $V = W$ on $\operatorname{supp} f$, $\int |f|^2 |\varphi|^2 W_1\,dx < \infty$ so $\varphi \in Q(\tilde{H})$. By (ii), $(\psi, H(f\varphi)) = (\psi, \tilde{H}(f\varphi))$ for all $\psi \in Q(H_0)$ so that $f\psi$, $(\nabla f)\psi$, $(-\Delta f)\psi \in Q(V_1)$. Since any $\psi \in Q(W_1)$ has this property, $H = \tilde{H}$. ▌

Theorem XI.32 Let H be a strongly semibounded local perturbation of $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let W be a function obeying:

(i) W is H_0-form bounded with relative bound $\alpha < 1$. Let $\tilde{H} = -\Delta + W$ be defined as a form sum.

(ii) $H = -\Delta + W$ outside the sphere of radius R, in the sense that if $f \in \mathscr{D}_{L\infty}$ has support in $\{x \mid |x| > R\}$, and $\varphi \in D(H)$ or $\varphi \in D(\tilde{H})$, then $f\varphi \in D(H) \cap D(\tilde{H})$ and $H(f\varphi) = \tilde{H}(f\varphi)$.

(iii) $\Omega^\pm(\tilde{H}, H_0)$ exist and are complete.

Then $\Omega^\pm(H, H_0)$ exist and are complete.

Proof By the chain rule and Proposition 3 of Section 3, it suffices to prove that $\Omega^\pm(H, \tilde{H})$ and $\Omega^\pm(\tilde{H}, H)$ exist. Let J be multiplication by a function in $\mathscr{D}_{L^\infty}$ that vanishes if $|x| < R$ and is 1 if $|x| > 2R$. Since $Q(H) \subset Q(H_0)$ and $Q(\tilde{H}) \subset Q(H_0)$, $(H + c)^{-1/2}(H_0 + 1)^{1/2}$ and $(\tilde{H} + c)^{-1/2}(H_0 + 1)^{1/2}$ are bounded for c sufficiently large. Thus $(1 - J)(H + c)^{-1/2}$ and $(1 - J) \times (\tilde{H} + c)^{-1/2}$ are in $\mathscr{I}_p$ if $p > \max\{n, 2\}$ by Theorem XI.20, and in particular are compact. Therefore $\Omega^\pm(H, \tilde{H}; 1 - J)$ and $\Omega^\pm(\tilde{H}, H; 1 - J)$ exist (and are in fact zero) by Lemma 2 of Section 3 and Problem 18. We are thus reduced to showing that $\Omega^\pm(H, \tilde{H}; J)$ and $\Omega^\pm(\tilde{H}, H; J)$ exist.

We claim that by mimicking the proof of Birman's theorem, it suffices to prove that, for any bounded interval I,

$$E_I(H)(HJ - J\tilde{H})E_I(\tilde{H}) \in \mathscr{I}_1 \tag{69}$$

For by hypothesis (ii), $JD(H) \subset D(\tilde{H})$, $JD(\tilde{H}) \subset D(H)$, so that the necessary subordinate condition holds: $(\tilde{H} + c)^{-1}J(H + c)$ and $(H + c)^{-1}J(\tilde{H} + c)$ are bounded. By (67) and hypothesis (ii), $(HJ - J\tilde{H})\varphi = -2\nabla \cdot (\nabla J)\varphi - (\Delta J)\varphi$ for $\varphi \in D(\tilde{H})$. Since $Q(H_0) \supset Q(H) \supset \operatorname{Ran} E_I(H)$, we have that $(E_I(H))\nabla$ is bounded. Thus, because ∇J, $\Delta J \in C_0^\infty$ and $(\tilde{H} + c)^\ell E_I(\tilde{H})$ is bounded, we need only prove that for some integer ℓ and any $g \in C_0^\infty$,

$$g(\tilde{H} + c)^{-\ell} \in \mathscr{I}_1 \tag{70}$$

By hypothesis (i), $(H_0 + c)^{1/2}(\tilde{H} + c)^{-1/2}$ is bounded. By Theorem XI.22,

$$g(H_0 + c)^{-1/2} \in \mathscr{I}_q \tag{71}$$

so long as $q > n$. Thus

$$g(\tilde{H} + c)^{-1/2} \in \mathscr{I}_q \tag{72}$$

for $q > n$. Let $A = (\tilde{H} + c)$ and $D = \partial_i$. We first claim that

$$gA^{-1} \quad \text{and} \quad DgA^{-1} \qquad \text{are in } \mathscr{I}_q \tag{73}$$

The first statement is obvious from (72) and the second follows from the boundedness of $DA^{-1/2}$, (72), and the calculation:

$$\begin{aligned} DgA^{-1} &= DA^{-1}g + D[A^{-1}, g] \\ &= DA^{-1}g + DA^{-1}DhA^{-1} + DA^{-1}fA^{-1} \end{aligned}$$

where $h = 2\nabla \cdot g$, $f = -\Delta g \in C_0^\infty$. A calculation similar to this shows that

$$\begin{aligned} gA^{-j-1} &= A^{-1}gA^{-j} + [g, A^{-1}]A^{-j} \\ &= A^{-1}gA^{-j} - A^{-1}DhA^{-j-1} - A^{-1}fA^{-j-1} \end{aligned} \tag{74}$$

It follows from (73), (74) that if $gA^{-j} \in \mathcal{I}_r$ for all $g \in C_0^\infty$, then $gA^{-j-1} \in \mathcal{I}_s$ for all $g \in C_0^\infty$ where $s^{-1} = \min\{1, r^{-1} + q^{-1}\}$. Thus starting with (73), we see inductively that for all $g \in C_0^\infty$, $gA^{-j} \in \mathcal{I}_{q_j}$ where $q_j = \min\{1, jq^{-1}\}$. Taking $\ell > q$, (70) holds. ▌

Corollary If $V = V_1 + V_2$ has compact support where $V_1 \geq 0$, $V_1 \in L^1$ and V_2 is $-\Delta$-form bounded with relative bound $\alpha < 1$, then $\Omega^\pm(-\Delta + V, -\Delta)$ exist and are complete.

The condition that $H_0 \leq c_1(H + c_2)$ is critical for the above results as the following spectacular example shows.

Thus far in this section we have presented a way of proving $\text{Ran}\,\Omega^+ = \text{Ran}\,\Omega^-$ that works in particular for $-\Delta + V$ with $V \in C_0^\infty(\mathbb{R}^3)$. We shall later discuss other methods of proving asymptotic completeness. Lest the reader think that asymptotic completeness must hold, we mention the existence of certain pathological examples:

Counterexample There exists a potential V that is bounded on compact subsets $\mathbb{R}^3\backslash\{0\}$ so that:

(i) V has compact support in $\mathbb{R}^3$.
(ii) $H = -\Delta + V$ is essentially self-adjoint on $D(-\Delta) \cap D(V)$.
(iii) $-\Delta + V$ is a positive operator.
(iv) The wave operators $\Omega^\pm = \text{s-lim}_{t \to \mp\infty}\, e^{itH}e^{-itH_0}$ exist.

but

(v) $\text{Ran}\,\Omega^+ \neq \text{Ran}\,\Omega^-$.

Let us describe the potential V which has been constructed by D. Pearson. There are basic building blocks of size $8(a + a^4)$ consisting of eight square wells as shown in Figure XI.3. Now define a_n by $8(a_n + a_n^4) = 2^{-n}$. The potential V will be a function W of $|\mathbf{r}|$. W will be 0 on $(1, \infty)$, and equal to the basic block potential with $a = a_{n+1}$ on $(2^{-n-1}, 2^{-n})$. Thus V is schema-

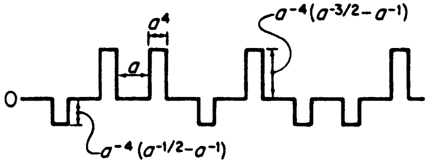


FIGURE XI.3 Pearson's building blocks.

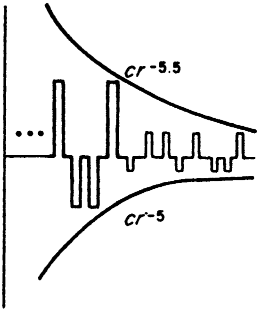


FIGURE XI.4 Schematic of Pearson's potential.

tically shown in Figure XI.4: It does not get larger than $cr^{-5.5}$ or smaller than $-cr^{-5}$, and its maximum oscillations approximately reach these curves. Notice also that it is "mostly" zero as $r \to 0$.

Physically, the reason for the breakdown of asymptotic completeness is that there exist incoming waves which in the future have two pieces, one of which scatters outward and another which gets trapped near the origin. Because of the positive bumps, the particle is prevented from reaching the origin in finite time, which is why H is essentially self-adjoint. The negative bumps prevent the particle from just bouncing off. We shall not prove the claimed properties for V, but refer the reader to the reference in the Notes.

To illustrate the wide applicability of the methods we have described, we consider two last examples, one a model of scattering from a thin slab of matter and the other of scattering from a semi-infinite chunk of matter.

Example 3 Let W be a function on $\mathbb{R}^3$ obeying

$$|W(x)| \le C_1(1 + |x|)^{-\alpha}$$

Fix k and let

$$V(x) = \sum_{\substack{n_1 = 0, \ldots, k \\ n_2, n_3 \in Z}} W(x_1 - n_1, x_2 - n_2, x_3 - n_3)$$

So long as $\alpha > 2$, the method of estimating sums by integrals easily shows that the sum converges and

$$|V(x)| \le C(1 + |x_1|)^{-(\alpha - 2)}$$

The wave operators $\Omega^{\pm}(-\Delta + V, -\Delta)$ describe the scattering of a single particle from an array of particles in a slab of $k + 1$ planes of scattering sites. If $\hat{u}$ is C^∞ with compact support away from points where $k_1 = 0$, it is easy to see that

$$\|Ve^{+it\Delta}u\|_2 \le (1 + |t|)^{-(\alpha - 2)}$$

by using stationary phase methods. It follows that, if $\alpha > 3$, $\Omega^{\pm}(-\Delta + V, -\Delta)$ will exist. Moreover, one can prove that $\operatorname{Ran} \Omega^+ = \operatorname{Ran} \Omega^-$ as follows: The function V is periodic in the 2 and 3 directions; and for that reason, $H = -\Delta + V$ has a (direct integral) decomposition as a fibered operator in the sense of Section XIII.16. The situation is somewhat different than that in Section XIII.16, where we discuss potentials periodic in all three directions. In that case the fibers are operators with purely discrete spectrum. In this case the fibers $H_0(k)$ for $-\Delta$ have purely absolutely continuous spectrum, and the fibers $H(k)$ have some absolutely continuous spectrum but also the possibility of some eigenvalues. One shows that $(H(k) + i)^{-1} - (H_0(k) + i)^{-1}$ is trace class for all k from which it follows that $\operatorname{Ran} \Omega^+(H, H_0) = \operatorname{Ran} \Omega^-(H, H_0) = \int^{\oplus} P_{\text{ac}}(H(k))\, dk$. For details in the above construction, the reader should consult the reference in the Notes. We remark that it may happen that the $H(k)$ have point spectrum contributing to absolutely continuous spectrum of H (as in Section XIII.16) in which case $\operatorname{Ran} \Omega^+ = \operatorname{Ran} \Omega^- \neq \operatorname{Ran} P_{\text{ac}}(H)$.

Example 4 Let W be a bounded periodic function on $\mathbb{R}$ and let $H_0 = -d^2/d^2x$, $H_1 = H_0 + W$. As we shall describe in Section XIII.16, H_1 is a model for the motion of an electron in a solid. Let

$$V(x) = \begin{cases} W(x), & x > 0 \\ 0, & x \leq 0 \end{cases}$$

so that $H = H_0 + V$ describes a model for electron scattering off a large (idealized as semi-infinite) chunk of solid. One expects that as $t \to \infty$ any solution $e^{-iHt}\varphi$ with $\varphi \in \operatorname{Ran} P_{\text{ac}}(H)$ should approach a sum of a free plane wave moving to the left and a solution $e^{-itH_1}\psi$ moving to the right in the solid. Let us prove this.

Let J be multiplication by a C^{∞} function φ on $\mathbb{R}$ that is 0 on $(-\infty, -1)$ and 1 on $(1, \infty)$. Then, as in the proof of Theorem XI.32, $E_I(A) \times (AJ - JB)E_I(B)$ is trace class for any of the five possibilities obtained as $\langle A, B\rangle$ run through $\langle H_0, H_0\rangle$, $\langle H_1, H_1\rangle$, $\langle H, H\rangle$, $\langle H, H_1\rangle$, $\langle H_1, H\rangle$, and the same is true if J is replaced by $1 - J$ and H_0 and H_1 are interchanged. Moreover, since $D(H_1) = D(H) = D(H_0)$ and $JD(H_0) \subset D(H_0)$, all pairs are mutually subordinate.

Now, for $B = H, H_1, H_0$, define

$$P_r^{\pm}(B) = \Omega^{\pm}(B, B; J), \qquad P_l^{\pm}(B) = \Omega^{\pm}(B, B; 1 - J)$$

where the limits exist by the above and Birman's theorem. Since $J^* = J$ and

$(J^2 - J)(B+1)^{-1}$ is compact, the $P^{\pm}_{\ell,\mathrm{r}}(B)$ are all orthogonal projections with

$$P^{\pm}_{\ell}(B) + P^{\pm}_{\mathrm{r}}(B) = P_{\mathrm{ac}}(B) \qquad \text{and} \qquad P^{\pm}_{\ell}(B)P^{\pm}_{\mathrm{r}}(B) = 0$$

by the intertwining relations for $\Omega^{\pm}(A, B; J)$. Moreover, Ran $P^{\pm}_{\ell}(B)$ is precisely the set of $\varphi \in$ Ran $P_{\mathrm{ac}}(B)$ so that $e^{-itB}\varphi$ moves off to $-\infty$ as $t \to \mp\infty$ in the sense that

$$\lim_{t \to \mp\infty} \int_a^{\infty} |(e^{-itB}\varphi)(x)|^2\, dx = 0$$

for any a.

Let

$$W^{\pm}_0 = \Omega^{\pm}(H, H_0; 1 - J), \qquad W^{\pm}_1 = \Omega^{\pm}(H, H; J)$$

Using the above results, it is not hard to show that these operators exist and that $W^{\pm}_0$ are a partial isometries with initial spaces $P^{\pm}_{\ell}(H_0)$ and final spaces $P^{\pm}_{\ell}(H)$. The same is true if W_0 is replaced by W_1, H_0 by H_1 and ℓ by r. Thus $P_{\mathrm{ac}}(H) = P^{\pm}_{\ell}(H) + P^{\pm}_{r}(H)$ implies that $P_{\mathrm{ac}}(H) =$ Ran $W^{\pm}_0 \oplus$ Ran $W^{\pm}_1$, which is the desired completeness statement.

An interesting consequence of the above is that if ψ is a vector with the support of $\hat{\psi}$ in (a, b) where $a > 0$ and (a^2, b^2) is inside a gap for H_1 (we shall show in Section XIII.16 that H_1 has spectrum $\bigcup_i [\alpha_i, \beta_i]$ with $\alpha_1 < \beta_1 \le \alpha_2 < \beta_2 \le \cdots$ where "typically" the "gaps" (β_i, α_{i+1}) are nonempty), then $W^{-}_0\psi \in$ Ran W^{+}_0; that is, a particle sent in at an energy in the gap is totally reflected. One can combine the above ideas with those in Example 3 and treat scattering from a half-space of higher dimensional crystal, or scattering from various kinds of crystal defects. These subjects and the details of the above construction are treated in the reference in the Notes.

We conclude this section with a formal definition and discussion of the scattering operator in two-body quantum mechanics. In interpreting experimental scattering data, the natural question is the following: We prepare a state that in the past looks like the state $e^{-iH_0t}\varphi$, and we want to know how it looks in the future, that is, we look at $e^{-iHt}\Omega^{+}\varphi$. We ask: What is the probability of finding that this state is the free state $e^{-iH_0t}\psi$ asymptotically in the future? By the rules of quantum mechanics, this probability $P_{\varphi\to\psi}$ is given by

$$\begin{aligned} P_{\varphi\to\psi} &= |(\Omega^{-}\psi, \Omega^{+}\varphi)|^2 \\ &= |(\psi, (\Omega^{-})^{*}\Omega^{+}\varphi)|^2 \end{aligned}$$

Definition If $\Omega^{\pm}$ exist, we define the **S-matrix, S-operator**, or scattering operator by

$$S = (\Omega^{-})^{*}\Omega^{+}$$

Notice that this definition makes sense even if Ran Ω^+ does not equal Ran Ω^-. While completeness is not needed to define S, it is equivalent to S being unitary.

We shall discuss S in detail in Sections 6 and 8. At this point, we note some simple properties of S (Problem 49).

Proposition

(a) $Se^{iH_0t} = e^{iH_0t}S$ for all t. S leaves $D(H_0)$ invariant; and if $\psi \in D(H_0)$, then $H_0(S\psi) = S(H_0\psi)$.
(b) If U is any unitary operator that commutes with H and H_0, then $US = SU$. In particular, if V is rotationally invariant, then S is rotationally invariant.
(c) $\overline{(S\psi)(x)} = (S^*\bar{\psi})(x)$.
(d) S is unitary if and only if Ran Ω^+ = Ran Ω^-.

(c) is called time reversal invariance for reasons discussed in the Notes.

On account of the continuity properties proved for the correspondence $A, B \mapsto \Omega^\pm(A, B)$ within the Kato–Birman theory, S has continuity properties. Typical is the following:

Proposition Let V_n and V_∞ be in $L^{3/2}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ and suppose that $\lim_{n\to\infty} \|V_n - V_\infty\|_1 = 0$ and $\sup_n \|V_n\|_{3/2} < \infty$. Let $S(V)$ be the S-matrix for $-\Delta + V$. Then

$$\operatorname*{s-lim}_{n\to\infty} S(V_n) = S(V_\infty)$$

Proof By mimicking the proof of Theorem XI.30, one sees (Problem 50) that $(H_n + i)^{-1} \to (H_\infty + i)^{-1}$ in trace class norm. Thus, by Problem 28,

$$\Omega^\pm(H_n, H_0) \to \Omega_\infty^\pm$$

strongly, so $S_n \to S$ weakly. But by completeness, the S_n and S are all unitary, so $S_n \to S$ strongly. ▌

There is one final property of $\Omega^\pm$ and S which we would like to discuss. We defer the full physical interpretation of this result until we prove a similar result for N-body systems, but we note that if we have scattering from a fixed scattering center and we take a fixed state and translate it toward infinity, it will miss the scattering center (see Figure XI.5).

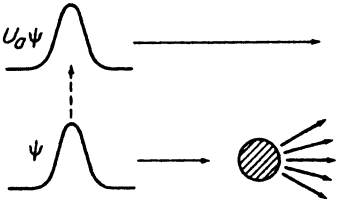


FIGURE XI.5 The cluster property.

Theorem XI.33 Under the hypotheses of Theorem XI.24

$$\operatorname*{s-lim}_{\mathbf{a}\to\infty} U_{\mathbf{a}}^{-1}\Omega^{\pm} U_{\mathbf{a}} = I$$

$$\operatorname*{s-lim}_{\mathbf{a}\to\infty} U_{\mathbf{a}}^{-1} S U_{\mathbf{a}} = I$$

where $U_{\mathbf{a}}$ are the operators $(U_{\mathbf{a}}f)(\mathbf{r}) = f(\mathbf{r}-\mathbf{a})$.

Proof We shall prove that $\text{s-lim}_{a\to+\infty} U_a^{-1}\Omega^{\pm}U_a = I$, from which it follows that $\text{w-lim}_{a\to\infty} U_a^{-1}SU_a = I$. Since $\|U_a S U_a^{-1}\| \le 1$, this implies that $\text{s-lim}_{a\to\infty} U_a^{-1}SU_a = I$.

By an $\varepsilon/3$ argument, we need only prove that

$$\lim_{a\to\infty} (U_a^{-1}(\Omega^{\pm} - 1)U_a)\varphi = 0$$

for all $\varphi \in \mathscr{S}$. For such φ,

$$U_a^{-1}(\Omega^{\pm} - 1)U_a\varphi = \mp i\int_0^{\mp\infty} (U_a^{-1}e^{iHt}Ve^{-iH_0t}U_a)\varphi\, dt$$

Let $F_a(t)$ denote $\|U_a^{-1}e^{-iHt}Ve^{-iH_0t}U_a\varphi\|$. It is easy to check that $F_a(t) = \|V_a e^{-iH_0t}\varphi\|$ where $V_a(r) = V(r+a)$. Looking at the second proof of Theorem XI.24, we see that $F_a(t)$ is bounded by an L^1 function of t uniformly in a because the L^p-norm of V_a is independent of a. By the dominated convergence theorem, it thus suffices to show that $F_a(t)\to 0$ for each fixed t. Since e^{-iH_0t} leaves $\mathscr{S}$ invariant, we need just show that $\lim_{a\to\infty}\|V_a\varphi\| = 0$ for all $\varphi\in\mathscr{S}$ and this is easy. ▮

XI.5 Quantum scattering II: *N*-body case

Scattering theory for N-body quantum systems is complicated for two reasons, one kinematical and one dynamical. The kinematic reason appears already for $N = 3$. Before one removes the center of mass one has a natural coordinate system $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$ in $\mathbb{R}^{3N} = \mathbb{R}^9$. Once we decide to take $\mathbf{R} = (\mu_1 + \mu_2 + \mu_3)^{-1}(\mu_1 \mathbf{r}_1 + \mu_2 \mathbf{r}_2 + \mu_3 \mathbf{r}_3)$ as a variable, there is no natural choice for the other six coordinates. For example, we have the pairs $\langle \mathbf{r}_{12}, \mathbf{r}_{13} \rangle$ or $\langle \mathbf{r}_{12}, \mathbf{r}_{23} \rangle$ or $\langle \mathbf{r}_{13}, \mathbf{r}_{23} \rangle$ where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Also, one might first change coordinates in the 1, 2 system to $\mathbf{R}_{12} = (\mu_1 + \mu_2)^{-1} \times (\mu_1 \mathbf{r}_1 + \mu_2 \mathbf{r}_2)$ and $\mathbf{r}_{12}$ and then go to the three-body system taking coordinates $\mathbf{R}$, $\mathbf{r}_{12}$, and $\zeta_2 = \mathbf{R}_{12} - \mathbf{r}_3$ (see Figure XI.6). The point is that various coordinates enter at various stages of the theory, and it is common to change coordinates in the middle of a proof. This kinematical complication is a nuisance.

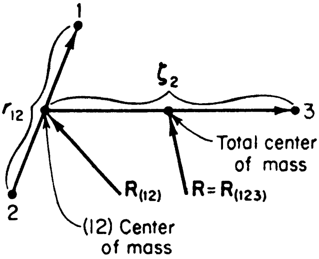


FIGURE XI.6 Jacobi coordinates, $N = 3$.

The dynamical complication involves the richness of different sorts of scattering phenomena possible even for a three-body system. Suppose that particles 1 and 2 can form a bound state. Then one not only expects scattering of the "free" particles 1, 2, 3 into free particles (elastic three-body scattering) but also **capture processes** where "free" particles 1, 2, 3 are sent in and a bound state of 1 and 2 together with a "free" particle 3 comes out. These processes are indicated schematically in Figure XI.7a and b. Similarly, one

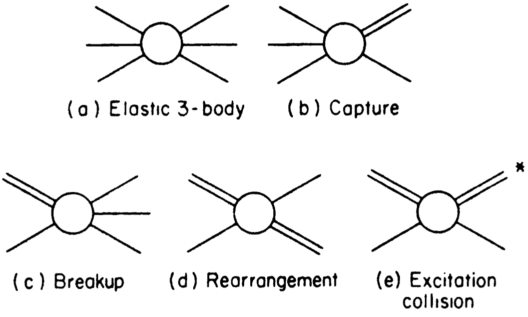


FIGURE XI.7 Three-body collision processes.

would like to describe **breakup processes** $(12) + 3 \to 1 + 2 + 3$ and **rearrangement collisions** $(12) + 3 \to 1 + (23)$ where (ij) represents a bound cluster of particles i and j. If there is more than one bound state of 1, 2, say (12) and $(12)^*$, one can have **excitation collisions** $(12) + 3 \to (12)^* + 3$.

In the three-body case, we shall first enumerate the bound states of (12), (23), and (13) and for each such bound state b consider a "scattering channel." Instead of describing states that are asymptotically a three-free-particles state, we consider states that asymptotically consist of 1 and 2 bound in state b and 3 moving freely relative to (12). In the N-body case, we need to consider clustering into disjoint subsets $C_1, \ldots, C_k$ and a scattering channel for each k-tuple of bound states of $C_1, \ldots, C_k$. One expects scattering between channels. This complication is subtle and beautiful.

We begin by describing various coordinate systems. Consider the Hamiltonians

$$\tilde{H} = -\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

$$\tilde{H}_0 = -\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_i$$

on $L^2(\mathbb{R}^{3N})$ where we write $\mathbf{r} = \langle \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle \in \mathbb{R}^{3N}$ and $-\Delta_i$ is the Laplacian in the $\mathbf{r}_i$ variables. We now change coordinates to $\mathbf{R} = (\sum_{i=1}^N \mu_i)^{-1} \times \sum_{i=1}^N \mu_i \mathbf{r}_i$ and $N - 1$ additional 3-vector coordinates $\xi_1, \ldots, \xi_{N-1}$. These coordinates are required to satisfy two additional conditions: First, for each $i \neq j$, $\mathbf{r}_i - \mathbf{r}_j$ is required to be a linear combination of the ξ_i. Secondly, the differential operator $\tilde{H}_0$, when written in the new coordinates, is required to have no terms of the form $\nabla_{\mathbf{R}} \cdot \nabla_{\xi_i}$. Actually, as we shall see, the first condition implies the second. Such a coordinate system defines a decomposition $L^2(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{3N-3})$ and a tensor decomposition of H and H_0:

$$\tilde{H} = h_0 \otimes 1 + 1 \otimes H$$

$$\tilde{H}_0 = h_0 \otimes 1 + 1 \otimes H_0$$

where $h_0 = -(2\sum_{i=1}^N \mu_i)^{-1}\Delta_{\mathbf{R}}$. The exact form of H depends on the coordinate system used for $\xi_1, \ldots, \xi_{N-1}$. As in the two-body case, one can think of a change of coordinates as an alternative description of the same operator or in terms of a unitary transformation. We shall take the former view. For some coordinate changes, the Jacobian will be a nonzero constant different from one, and it must thus be included in the inner product.

We consider three specific kinds of coordinate changes:

Atomic coordinates Let $\boldsymbol{\eta}_i = \mathbf{r}_i - \mathbf{r}_N$. Then

$$H_0 = -\sum_{i=1}^{N-1} (2m_{iN})^{-1}\Delta_i + \sum_{i<j} (\mu_N)^{-1}\nabla_i \cdot \nabla_j$$

where $(m_{iN})^{-1} = \mu_i^{-1} + \mu_N^{-1}$, $\Delta_i = \Delta_{\eta_i}$, and $\nabla_i = \nabla_{\eta_i}$. Moreover,

$$H = H_0 + \sum_{i=1}^{N-1} V_{iN}(\boldsymbol{\eta}_i) + \sum_{i<j<N} V_{ij}(\boldsymbol{\eta}_i - \boldsymbol{\eta}_j)$$

The reader is asked to carry through these computations in Problems 52a. As the name suggests, this coordinate system is especially useful in systems where one particle is distinguished from the others, such as atomic systems where the nucleus is distinguished. The additional terms $\sum_{i<j} \mu_N^{-1}\nabla_i \cdot \nabla_j$ are often a nuisance. They are called **Hughes–Eckart terms.** Notice that there are no cross terms in $\tilde{H}_0$ between $\mathbf{R}$ and $\boldsymbol{\eta}_i$: It follows that for any choice of the ξ_i satisfying the first requirement above, the second requirement will automatically hold.

Jacobi coordinates Let

$$\zeta_i = \mathbf{r}_{i+1} - \left(\sum_{j\le i} \mu_j\right)^{-1}\left(\sum_{j\le i} \mu_j \mathbf{r}_j\right), \qquad i = 1, \ldots, N-1$$

Then (Problem 52b)

$$H_0 = -\sum_{i=1}^{N-1} (2\nu_i)^{-1}\Delta_{\zeta_i}$$

where $\nu_i^{-1} = \mu_{i+1}^{-1} + (\sum_{j\le i} \mu_j)^{-1}$ and $H = H_0 + \sum_{i<j} V_{ij}(\mathbf{r}_{ij})$ where $\mathbf{r}_{ij}$ is shorthand for $\mathbf{r}_i - \mathbf{r}_j$ written in terms of the ζ_j; for example,

$$\mathbf{r}_{41} = \zeta_3 + \frac{\mu_3}{\mu_1 + \mu_2 + \mu_3}\zeta_2 + \frac{\mu_2}{\mu_1 + \mu_2}\zeta_1$$

Jacobi coordinates are obtained by first changing variables from $\langle \mathbf{r}_1, \mathbf{r}_2 \rangle$ to $\zeta_1 = \mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{R}_{(12)} = (\mu_1 + \mu_2)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2)$, then from $\langle \mathbf{R}_{(12)}, \mathbf{r}_3 \rangle$ to $\zeta_2 = \mathbf{r}_3 - \mathbf{R}_{(12)}$, and $\mathbf{R}_{(123)} = (\mu_1 + \mu_2 + \mu_3)^{-1}[(\mu_1 + \mu_2)\mathbf{R}_{(12)} + \mu_3\mathbf{r}_3]$, and so forth (see Figure XI.6). At each stage, one pair of variables is changed to a two-body center of mass and a relative coordinate. Since there are no cross terms in the change to center of mass coordinates for two-body systems, there are no Hughes–Eckart terms in the N-body H_0 above, which is the virtue of Jacobi coordinates. The disadvantage of Jacobi coordinates is the complicated form of $\mathbf{r}_{ij}$, although $\mathbf{r}_{12} = -\zeta_1$ is simple. Given any permutation $\langle i_1, \ldots, i_N \rangle$ of $\langle 1, \ldots, N \rangle$, there is an associated Jacobi coordinate system in which $\mathbf{r}_{i_1 i_2}$ is simple.

Clustered Jacobi coordinates The last coordinate system we discuss is particularly useful for scattering theory. In order to describe the breakup of an N-body system into bound clusters, we introduce some formal definitions and notation which will play an important role in this section and Section XIII.5.

Definition A partition D of $\{1, \ldots, N\}$ into k disjoint subsets $C_1, \ldots, C_k$ whose union is $\{1, \ldots, N\}$ is called a **cluster decomposition**. If $D = \{C_1, \ldots, C_k\}$ is a cluster decomposition and i, j are two numbers in $\{1, \ldots, N\}$, we write iDj if and only if i and j are in the same cluster C_ℓ and $\sim iDj$ if they are in different clusters. The symbols $\sum_{iDj}$ and $\sum_{\sim iDj}$ represent the sum over those pairs $\langle i, j\rangle$ with $i < j$ obeying iDj or $\sim iDj$, respectively.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. Let

$$\tilde{H}(C_\ell) = -\sum_{i \in C_\ell} (2\mu_i)^{-1}\Delta_i + \sum_{i<j,\, i,\, j \in C_\ell} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

and define $H(C_\ell)$, the **cluster Hamiltonian**, to be $\tilde{H}(C_\ell)$ with its center of mass removed.

$H(C_\ell)$ is an operator in $L^2(\mathbb{R}^{3N-3})$; it is independent of coordinates in the other clusters so $H(C_\ell) = h_{C_\ell} \otimes 1$ if we decompose $L^2(\mathbb{R}^{3N-3})$ as $L^2(\mathbb{R}^{3n_\ell-3}) \otimes L^2(\mathbb{R}^{3N-3n_\ell})$ where n_ℓ is the number of elements in C_ℓ. We shall henceforth use the symbol $H(C_\ell)$ for both the operator on $L^2(\mathbb{R}^{3N-3})$ and the operator on $L^2(\mathbb{R}^{3n_\ell-3})$ which we denoted above as h_{C_ℓ}. When we wish to emphasize which operator is intended, we shall talk about "$H(C_\ell)$ as an operator on $\mathscr{H}$" or "$H(C_\ell)$ as an operator on $\mathscr{H}_{C_\ell}$" where $\mathscr{H}_{C_\ell}$ is the space $L^2(\mathbb{R}^{3n_\ell-3})$ of functions of the internal coordinates of the cluster C_ℓ.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. The **intercluster potential** I_D is defined by

$$I_D = \sum_{\sim iDj} V_{ij}$$

Thus I_D is the sum of interactions between particles in different clusters.

Definition Let $D = \{C_\ell\}_{\ell=1}^k$ be a cluster decomposition. Let $\tilde{H}_D = \tilde{H} - I_D = \sum_{\ell=1}^k \tilde{H}(C_\ell)$ and define the **cluster decomposition Hamiltonian** H_D as the Hamiltonian $\tilde{H}_D$ with its center of mass removed. Thus

$$H_D = H - I_D$$

Since I_D depends only on coordinate differences $r_i - r_j$, it is unaffected by removal of the center of mass.

Notice that $H_D \neq \sum_{\ell=1}^k H(C_\ell)$; rather $H_D = T_D + \sum_{\ell=1}^k H(C_\ell)$ where T_D is the kinetic energy of the center of masses of the individual clusters with the total center of mass energy removed. Thus corresponding to the partition of the $3N-3$ coordinates in the k sets of internal coordinates for $C_1, \ldots, C_k$ plus the set of $3(k-1)$ coordinates describing the relative positions of the centers of mass of the clusters $\{C_i\}_{i=1}^k$, the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^{3N-3})$ is written as

$$\mathscr{H} = \mathscr{H}_D \otimes \mathscr{H}_{C_1} \otimes \mathscr{H}_{C_2} \otimes \cdots \otimes \mathscr{H}_{C_\ell}$$

and

$$\begin{aligned} T_D &= t_D \otimes 1 \otimes \cdots \otimes 1 \\ H(C_1) &= 1 \otimes h_{C_1} \otimes 1 \otimes \cdots \otimes 1 \\ &\vdots \\ H(C_\ell) &= 1 \otimes 1 \otimes \cdots \otimes h_{C_\ell} \end{aligned}$$

Clustered Jacobi coordinates are chosen precisely to make T_D simple. To obtain these coordinates we first change from $\langle \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle$ to

$$\langle \mathbf{R}_1, \ldots, \mathbf{R}_k, \xi_1^{(C_1)}, \ldots, \xi_{n_1-1}^{(C_1)}, \ldots, \xi_{n_k-1}^{(C_k)} \rangle$$

where

$$\mathbf{R}_\ell = \left(\sum_{i \in C_\ell} \mu_i \right)^{-1} \sum_{i \in C_\ell} \mu_i \mathbf{r}_i$$

and $\xi_1^{(C_\ell)}, \ldots, \xi_{n_\ell-1}^{(C_\ell)}$ are coordinates which together with the $\mathbf{R}_\ell$ form a set of coordinates for C_ℓ. For example, we could fix some $j \in C_\ell$ and let $\{\xi_m^{(C_\ell)}\}_{m=1}^{n_\ell-1} = \{\mathbf{r}_i - \mathbf{r}_j\}_{i \in C_\ell;\, i \neq j}$. Thus $H(C_\ell)$ is a differential operator in the variables $\xi_m^{(C_\ell)}$. Therefore

$$\tilde{H} = \sum_{\ell=1}^k (-2m_{C_\ell})^{-1} \Delta_{R_\ell} + \sum_{\ell=1}^k H(C_\ell) + I_D$$

where $m_{C_\ell} = \sum_{i \in C_\ell} \mu_i$. Now treat $\mathbf{R}_1, \ldots, \mathbf{R}_\ell$ as a set of k-body variables and take Jacobi coordinates $\{\zeta_\ell\}_{\ell=1}^{k-1}$ for $\langle \mathbf{R}_1, \ldots, \mathbf{R}_k \rangle$ as the first $k-1$ coordinates of a new coordinate system; $\{\xi_m^{(C_\ell)}\}$, where $1 \leq m \leq n_\ell - 1$ and $1 \leq \ell \leq k$, as the next $N-k$ coordinates and then the center of mass as the last coordinate. Then

$$H_D = \sum_{\ell=1}^{k-1} (-2M_\ell)^{-1} \Delta_{\zeta_\ell} + \sum_{\ell=1}^k H(C_\ell)$$

where $M_\ell^{-1} = m_{C_{\ell+1}}^{-1} + (\sum_{k \le \ell} m_{C_k})^{-1}$. Thus we have a coordinate system in which H_D has a very simple form. The individual terms in the two sums depend on independent coordinates and thus commute with one another. Notice also that if $i \in C_1$, $j \in C_2$, then $\mathbf{r}_i - \mathbf{r}_j = -\zeta_1 + \xi_i^{(C_1)} - \xi_j^{(C_2)}$ where $\xi_i^{(C_\ell)}$ is some combination of internal coordinates for C_ℓ which gives the distance of $\mathbf{r}_i$ from the center of mass of the cluster C_ℓ.

To see how these definitions operate, let us consider the simplest nontrivial example:

Example (clustered Jacobi coordinates) Let $N = 5$ and consider the partition $D = \{C_1, C_2, C_3\}$, $C_1 = \{1, 2, 3\}$, $C_2 = \{4\}$, $C_3 = \{5\}$. Then

$$\mathbf{R}_1 = (\mu_1 + \mu_2 + \mu_3)^{-1}(\mu_1\mathbf{r}_1 + \mu_2\mathbf{r}_2 + \mu_3\mathbf{r}_3)$$

$$\xi_1^{(C_1)} = \mathbf{r}_1 - \mathbf{r}_3, \qquad \xi_2^{(C_1)} = \mathbf{r}_2 - \mathbf{r}_3$$

$$\mathbf{R}_2 = \mathbf{r}_4, \qquad \mathbf{R}_3 = \mathbf{r}_5, \qquad \zeta_1 = \mathbf{R}_2 - \mathbf{R}_1$$

$$\zeta_2 = \mathbf{R}_3 - (\mu_1 + \mu_2 + \mu_3 + \mu_4)^{-1}[(\mu_1 + \mu_2 + \mu_3)\mathbf{R}_1 + \mu_4\mathbf{R}_2]$$

The clustered Jacobi coordinates are just $\langle \zeta_1, \zeta_2, \xi_1^{(C_1)}, \xi_2^{(C_1)} \rangle$. See Figure XI.8. As an example of how $\mathbf{r}_{ij}(i \in C_1, j \in C_2)$ appears, notice that

$$\mathbf{r}_4 - \mathbf{r}_3 = \zeta_1 + (\mu_1 + \mu_2 + \mu_3)^{-1}[\mu_1\xi_1^{(C_1)} + \mu_2\xi_2^{(C_1)}]$$

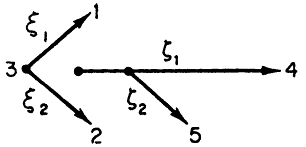


FIGURE XI.8 Clustered Jacobi coordinates, $N = 5$.

Having completed our discussion of the kinematics of N-body systems, we turn to the existence questions of scattering theory. We use the same technical ideas as in the two-body theory with the usual two complications. First, kinematics makes the notation more complex and the reader should keep a cool head; secondly, the wealth of scattering phenomena will require us to look at more objects than just s-$\lim_{t \to \mp\infty} e^{+iHt}e^{-iH_0t}$. For suppose that $\psi = \lim_{t \to +\infty} e^{+iHt}e^{-iH_0t}\varphi$. Then $e^{-iHt}\psi$ approaches $e^{-iH_0t}\varphi$ as $t \to +\infty$ and it looks like a state with N freely moving particles. If we want to describe states that asymptotically look like bound clusters $C_1, \ldots, C_k$ moving freely, we want $e^{-iHt}\psi$ to look like $e^{-iAt}\psi$ where A describes bound clusters moving freely. A must therefore include the forces that bind the clusters but should not have the forces between clusters. Thus we will take $A = H_D$, $D = \{C_1, \ldots, C_k\}$ and study a particular limit.

Definition Let H be the Hamiltonian of an N-body system with center of mass removed. Let $D = \{C_1, \ldots, C_k\}$ be a cluster decomposition of $\{1, \ldots, N\}$. If $\Omega_D^{\pm} = \text{s-lim}_{t \to \mp\infty} e^{+iHt}e^{-iH_D t}$ exist, we say that the **clustered channel wave operators exist.**

Theorem XI.34 (Hack's theorem) Let

$$H = \sum_{i=1}^{N-1} (-2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(\mathbf{r}_{ij})$$

where each $V_{ij} \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ with $2 < p < 3$. Then the clustered channel wave operators $\Omega_D^{\pm}$ exist for each cluster decomposition D.

Proof The basic structure of the proof is exactly that of the second proof of Theorem XI.24. Choose a clustered Jacobi coordinate system with coordinates $\zeta_1, \ldots, \zeta_{k-1}; \xi_1^{(C_1)}, \ldots, \xi_{n_1-1}^{(C_1)}; \ldots \xi_{n_k-1}^{(C_k)}$ where $\{\xi^{(C_\ell)}\}$ is a family of internal coordinates for cluster C_ℓ and $\{\zeta\}$ are the Jacobi coordinates for the motion of the centers of mass of the clusters. Consider the set

$$\begin{aligned}\mathscr{D}_D = \{\varphi(\zeta_1, \ldots, \zeta_{k-1})\eta_1(\xi^{(C_1)}) \cdots \eta_k(\xi^{(C_k)}) \mid \varphi \in \mathscr{S}(\mathbb{R}^{3k-3}),\\ \text{and} \quad \eta_\ell \in D(H(C_\ell)), \|\eta_\ell\| = 1\}\end{aligned}$$

Finite linear combinations of vectors in $\mathscr{D}_D$ are dense, so we need only prove that $\lim_{t \to \mp\infty} e^{+iHt}e^{-iH_D t}\psi$ exists for all $\psi \in \mathscr{D}_D$.

By Cook's method, it is sufficient to show that

$$\left\| \frac{d}{dt}(e^{+iHt}e^{-iH_D t}\psi) \right\| = \|I_D e^{-iH_D t}\psi\|$$

is in $L^1(\pm 1, \pm\infty)$ for all $\psi \in \mathscr{D}_D$. Since I_D is a finite sum, it is enough to show $\|V_{ij}e^{-iH_D t}\psi\| \in L^1(\pm 1, \pm\infty)$ for each i, j with $\sim iDj$. Since each V_{ij} is a sum of two terms, one in L^2 the other in L^r, we can suppose V_{ij} is in either L^2 or L^r $(2 < r < 3)$ and use the triangle inequality to estimate the sum. Given i, j, we shall pick the Jacobi coordinates so that $\zeta_1 = R_a - R_b$ where $i \in C_a$, $j \in C_b$. Since change of Jacobi coordinates of $\langle R_1, \ldots, R_k\rangle$ by reordering leaves $\mathscr{S}(\mathbb{R}^{3k-3})$ invariant, there is no problem with the fact that we must change the meaning of "ζ_ℓ" as we vary i and j.

We next note that the individual terms in

$$H_D = \sum_{\ell=1}^{k-1}(-2M_\ell)^{-1}\Delta_\ell + \sum_{\ell=1}^{k} H(C_\ell)$$

commute, so

$$e^{-itH_D} = \left(\prod_{\ell=1}^{k-1} e^{+it(2M_\ell)^{-1}\Delta_\ell}\right) \prod_{\ell=1}^{k} e^{-itH(C_\ell)}$$

Moreover, V_{ij} depends only on ζ_1 and internal coordinates from C_1, C_2, so V_{ij} commutes with $e^{is\Delta_\ell}$, $\ell \neq 1$ and $e^{-itH(C_\ell)}$, $\ell \neq 1, 2$. Thus

$$\|V_{ij} e^{-itH_D}\psi\| = \left\| V_{ij}(e^{is\Delta_1}\varphi)(\eta_{1,t})(\eta_{2,t}) \prod_{\ell=3}^{k} \eta^{(C_\ell)} \right\|$$

where $s = t(2M_1)^{-1}$; and $\eta_{\ell,t} = e^{-iH(C_\ell)t}\eta_\ell$. V_{ij} depends only on ζ_1 and coordinates in C_1 and C_2, so

$$\|V_{ij} e^{-itH_D}\psi\| = \|V_{ij}(e^{is\Delta_1}\varphi)(\eta_{1,t})(\eta_{2,t})\|_{C_1, C_2; \zeta}$$

where the symbol $\|\cdot\|_{C_1, C_2; \zeta}$ means the L^2-norm integrating over the variables $\xi^{(C_1)}$, $\xi^{(C_2)}$, and ζ. Thus

$$\|V_{ij} e^{-itH_D}\psi\|^2 = \int F(\zeta_2, \ldots, \zeta_{k-1}; t)\, d\zeta_2 \cdots d\zeta_{k-1}$$

where

$$F(\zeta_2, \ldots, \zeta_{k-1}; t) = \int |V_{ij}^{(t)}(\zeta_1)|^2 |e^{is\Delta_1}\varphi(\zeta_1, \ldots, \zeta_{k-1})|^2\, d\zeta_1$$

and

$$|V_{ij}^{(t)}(\zeta_1)|^2 = \int |\eta_{1,t}(\xi_1^{(C_1)})|^2 |\eta_{2,t}(\xi_1^{(C_2)})|^2 |V_{ij}(\zeta_1 - \xi_i^{(C_1)} - \xi_j^{(C_2)})|^2\, d\xi^{(C_1)}\, d\xi^{(C_2)}$$

If we do all the $\xi^{(C_1)}$, $\xi^{(C_2)}$ integrations in the last integral except for the $\xi_i^{(C_1)} + \xi_j^{(C_2)}$ integration, we see that $|V_{ij}^{(t)}|^2$ is a convolution of $|V_{ij}|^2 \in L^{r/2}$ and a function in L^1 with L^1-norm $(\|\eta_{1,t}\|_2 \|\eta_{2,t}\|_2)^2 = 1$. Thus by Young's inequality, $\|V_{ij}^{t}\|_r \leq \|V_{ij}\|_r$. As a result of this estimate and the wave packet spreading of $e^{is\Delta_1}$, we conclude that

$$0 \leq F(\zeta_2, \ldots, \zeta_{k-1}) \leq \|V_{ij}^{(t)}\|_r^2 (s^{-\frac{3}{2}+3/p})^2 \int |\varphi(\zeta_1, \ldots, \zeta_{k-1})|^2\, d\zeta_1$$

where p is as given in Theorem XI.24 and in particular $p > 6$. Finally, we conclude that

$$\|V_{ij} e^{-itH}\psi\|^2 \leq [\|V_{ij}\|_r s^{-\frac{3}{2}+3/p} \|\varphi\|_2]^2$$

and thus $\|V_{ij} e^{-itH}\psi\| \in L^1(\pm 1, \pm\infty)$. This concludes the proof. ▌

The point of the above proof is that it reduces the existence problem for the N-body case to the same estimates we used in the two-body case. By using the form ideas discussed in the proof of Theorem XI.26 and the form version of Cook's method (Theorem XI.6), one easily obtains:

Theorem XI.35 Let

$$H = \sum_{i=1}^{N-1} (-2\mu_i)^{-1}\Delta_i + \sum_{i<j} V_{ij}(r_{ij})$$

on $L^2(\mathbb{R}^{(N-1)n})$. Suppose that each V_{ij} obeys

$$(1 + |r|^2)^{\frac{1}{2}+\varepsilon} V_{ij}(r) \in L^p(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$$

where $p = \frac{1}{2}n$ if $n \geq 3$; $p = 1$ if $n = 1$; and $p > 1$ if $n = 2$. Then the clustered channel wave operators $\Omega_D^\pm$ exist for each cluster decomposition D.

We now know that $\Omega_D^\pm$ exist and would like to construct scattering states. Not every $\psi = \Omega_D^- \kappa$ describes a state that approaches a system of bound clusters $\{C_1, C_2, \ldots, C_k\}$ moving freely relative to one another as $t \to \infty$. All we know is that $e^{-iHt}\psi$ and $e^{-iH_Dt}\kappa$ approach one another. But since $\text{s-lim}_{t\to\infty} e^{+iH_Dt}e^{-iH_0t}$ exists, if $\kappa = \lim_{t\to\infty} e^{+iH_Dt}e^{-iH_0t}\eta$, then $e^{-iHt}\psi$ and $e^{-iH_0t}\eta$ also look like one another as $t \to \infty$. The point is that for ψ to look like bound clusters as $t \to \infty$, it is not enough to have $e^{-itH}\psi - e^{-itH_D}\kappa \to 0$ for an arbitrary κ. κ must have the form $\kappa(\zeta, \xi^{(C_1)}, \ldots, \xi^{(C_k)}) = \varphi(\zeta)\eta_1(\xi^{(C_1)}) \cdots \eta_k(\xi^{(C_k)})$ where each η_ℓ is a bound state of $H(C_\ell)$. We thus are motivated to define:

Definition A **channel** is a cluster decomposition $D = \{C_1, \ldots, C_k\}$ together with functions $\eta_\ell \in \mathscr{H}_\ell$ such that each η_ℓ is an eigenfunction of $H(C_\ell)$ with eigenvalue E_ℓ. We shall use the symbols α, β, ... to stand for a channel and sometimes write

$$\alpha = \begin{pmatrix} C_1 & C_2 & \cdots & C_k \\ \eta_1 & \eta_2 & \cdots & \eta_k \end{pmatrix}$$

The eigenvalues $E_1, \ldots, E_k$ will be denoted $\{E_i^{(\alpha)}\}_{i=1}^k$ and are called **channel eigenenergies**. The cluster decomposition D associated with a channel α will be denoted by $D(\alpha)$.

Two channels where the η_ℓ differ by complex multiples are not considered distinct. Thus a channel is more accurately a cluster decomposition together with "rays of eigenfunctions." If C_ℓ contains only one particle, then we write $\mathscr{H}_{C_\ell} = \mathbb{C}$ (there are no internal coordinates), $H(C_\ell) \equiv 0$, η_ℓ is the element $1 \in \mathbb{C}$, and $E_\ell^{(\alpha)} = 0$.

Important Proviso In listing all channels $\alpha = \left(\begin{smallmatrix} C_1 & \cdots & C_k \\ \eta_1 & \cdots & \eta_k \end{smallmatrix}\right)$, we first make preliminary choices if some $H(C_\ell)$ has a degenerate eigenvalue. Explicitly, if E_0 is an eigenvalue of $H(C_\ell)$ of multiplicity n, we first pick n orthonormal functions in $\{\eta \mid H(C_\ell)\eta = E_0 \eta\}$ and then require that for any α with $E_\ell^{(\alpha)} = E_0$, η_ℓ is one of these n functions. Thus if α and β are distinct channels, either $D(\alpha) \neq D(\beta)$ or $D(\alpha) = D(\beta)$ and for some ℓ, $\eta_\ell^{(\alpha)}$ is orthogonal to $\eta_\ell^{(\beta)}$.

Definition Let α be a channel. Choose clustered Jacobi coordinates for the decomposition $D(\alpha)$, say $\langle \zeta_1, \ldots, \zeta_{k-1}, \xi_1^{(C_1)}, \ldots, \xi_{n_k-1}^{(C_k)} \rangle$. Call $\mathscr{H}_\alpha = L^2(\mathbb{R}^{3k-3})$ the **channel Hilbert space**, and define $\mathscr{T}_\alpha \colon \mathscr{H}_\alpha \to \mathscr{H} = L^2(\mathbb{R}^{3N-3})$, **the channel embedding** by

$$(\mathscr{T}_\alpha \varphi)(\zeta, \xi^{(C_\ell)}) = \varphi(\zeta_1, \ldots, \zeta_{k-1}) \prod_{\ell=1}^{k} \eta_\ell(\xi^{(C_\ell)})$$

The **channel wave operators** $\Omega_\alpha^\pm \colon \mathscr{H}_\alpha \to \mathscr{H}$ are defined by

$$\Omega_\alpha^\pm = \Omega_{D(\alpha)}^\pm \mathscr{T}_\alpha$$

The **channel Hamiltonian** H_α on $\mathscr{H}_\alpha$ is defined by

$$H_\alpha = H_\alpha^{(0)} + \sum_{\ell=1}^{k} E_\ell^{(\alpha)}$$

where $H_\alpha^{(0)} = \sum_{\ell=1}^{k-1} (-2M_\ell)^{-1} \Delta_\ell$ in Jacobi coordinates.

The wave operators $\Omega_\alpha^\pm$ have a simple direct physical interpretation. For, if $\psi = \Omega_\alpha^\pm \varphi$, then $e^{-iHt}\psi$ approaches $(e^{-iH_\alpha^{(0)}t}\varphi)(\prod_{\ell=1}^{k} e^{-itE_\ell^{(\alpha)}}\eta_\ell)$ as $t \to \mp\infty$. But $(e^{-iH_\alpha^{(0)}t}\varphi)(\prod_{\ell=1}^{k} e^{-iE_\ell^{(\alpha)}t}\eta_\ell)$ is precisely the wave function of bound clusters η_k moving freely relative to one another. Given this physical interpretation, we expect that Ran $\Omega_\alpha^\pm$ should be orthogonal to Ran $\Omega_\beta^\pm$. We have thus removed the multiple counting of asymptotic states that occurs in $\{\text{Ran } \Omega_D^\pm\}$. Before proving that Ran $\Omega_\alpha^\pm$ and Ran $\Omega_\beta^\pm$ are orthogonal if $\alpha \neq \beta$, we combine the channels.

Definition Let $\mathscr{C}$ be the collection of all channels with the proviso discussed above in case some $H(C_\ell)$ has a degenerate eigenvalue. Define the **asymptotic Hilbert space** $\mathscr{H}_{\text{asym}} = \bigoplus_{\alpha \in \mathscr{C}} \mathscr{H}_\alpha$, the **"free" Hamiltonian** H_{asym}

on $\mathscr{H}_{\text{asym}}$ by $H_{\text{asym}} = \bigoplus_{\alpha\in\mathscr{C}} H_\alpha$, the **embedding transformation** $\mathscr{T}\colon \mathscr{H}_{\text{asym}} \to \mathscr{H}$ by $\mathscr{T} = \bigoplus_{\alpha\in\mathscr{C}} \mathscr{T}_\alpha$, and the **wave operators** $\Omega^\pm\colon \mathscr{H}_{\text{asym}} \to \mathscr{H}$ by $\Omega^\pm = \bigoplus_{\alpha\in\mathscr{C}} \Omega_\alpha^\pm$. Let $\mathscr{H}_\pm = \text{Ran}\,\Omega^\pm$.

Theorem XI.36 Suppose that the cluster channel wave operators exist. Then:

(a) $\Omega^\pm = \text{s-lim}_{t\to\mp\infty}\, e^{+iHt}\mathscr{T}e^{-iH_{\text{asym}}t}$.
(b) (Orthogonality of channels) If $\alpha \neq \beta$, then $\text{Ran}\,\Omega_\alpha^\pm$ is orthogonal to $\text{Ran}\,\Omega_\beta^\pm$.
(c) $\Omega^\pm$ are isometries from $\mathscr{H}_{\text{asym}}$ to $\mathscr{H}$.
(d) $e^{iHt}\Omega^\pm = \Omega^\pm e^{iH_{\text{asym}}t}$.
(e) $\mathscr{H}_\pm \subset \mathscr{H}_{\text{ac}}(H)$.

Proof (a) This is a direct consequence of $e^{-iH_{D(\alpha)}t}\mathscr{T}_\alpha = \mathscr{T}_\alpha e^{-iH_\alpha t}$.

(b) Let $\varphi_\alpha \in \mathscr{H}_\alpha$, $\varphi_\beta \in \mathscr{H}_\beta$. Then $\Omega_\alpha^\pm\varphi_\alpha = \text{s-lim}_{t\to\mp\infty}\, e^{+iHt}\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha$ and similarly for φ_β. Thus since e^{+iHt} is unitary, it is sufficient to prove that $\lim_{t\to\mp\infty}(\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha, \mathscr{T}_\beta e^{-iH_\beta t}\varphi_\beta) = 0$ in order to conclude that $(\Omega_\alpha^\pm\varphi_\alpha, \Omega_\beta^\pm\varphi_\beta) = 0$. This is done by considering separately the cases where $D(\alpha) = D(\beta)$ and $D(\alpha) \neq D(\beta)$.

First suppose that $D(\alpha) = D(\beta)$. Then

$$\begin{aligned}(\mathscr{T}_\alpha e^{-iH_\alpha t}\varphi_\alpha, \mathscr{T}_\beta e^{-iH_\beta t}\varphi_\beta) &= (e^{-iH_{D(\alpha)}t}\mathscr{T}_\alpha\varphi_\alpha, e^{-iH_{D(\beta)}t}\mathscr{T}_\beta\varphi_\beta)\\ &= (\mathscr{T}_\alpha\varphi_\alpha, \mathscr{T}_\beta\varphi_\beta) = \left(\varphi_\alpha \prod_{\ell=1}^{k}\eta_\ell^{(\alpha)}, \varphi_\beta \prod_{\ell=1}^{k}\eta_\ell^{(\beta)}\right)\\ &= (\varphi_\alpha, \varphi_\beta)\left[\prod_{\ell=1}^{k}(\eta_\ell^{(\alpha)}, \eta_\ell^{(\beta)})\right] = 0\end{aligned}$$

because some $(\eta_\ell^{(\alpha)}, \eta_\ell^{(\beta)}) = 0$ by our proviso on degenerate eigenvalues.

Now suppose that $D(\alpha) \neq D(\beta)$. Let $E = \sum_{\ell=1}^{k_\beta} E_\ell^{(\beta)} - \sum_{\ell=1}^{k_\alpha} E_\ell^{(\alpha)}$. Then

$$\begin{aligned}(\mathscr{T}_\alpha e^{-itH_\alpha}\varphi_\alpha, \mathscr{T}_\beta e^{-itH_\beta}\varphi_\beta) &= e^{-itE}(\mathscr{T}_\alpha e^{-itH_\alpha{}^{(0)}}\varphi_\alpha, \mathscr{T}_\beta e^{-itH_\beta{}^{(0)}}\varphi_\beta)\\ &= e^{-itE}(\mathscr{T}_\alpha\varphi_\alpha, e^{-it[H_\beta{}^{(0)} - H_\alpha{}^{(0)}]}\mathscr{T}_\beta\varphi_\beta)\end{aligned}$$

$H_\beta^{(0)} - H_\alpha^{(0)} \neq 0$ because $D(\alpha) \neq D(\beta)$. Written in terms of Fourier transforms, $H_\beta^{(0)} - H_\alpha^{(0)}$ is multiplication by some function $f_{\alpha\beta}(p)$ which is a quadratic form in p and so has the form $f_{\alpha\beta}(p) = \sum_{i=1}^{3N-3} a_i p_i^2$ for some coordinate system, with some $a_i \neq 0$. Renumber the p_i so that

$a_1, \ldots, a_m \neq 0; a_{m+1} = a_{m+2} = \cdots = 0$. Let ψ_1 and ψ_2 be in $\mathscr{S}(\mathbb{R}^{3N-3})$. Then by (IX.31),

$$\begin{aligned}(\psi_1, e^{-it(H_\beta(0) - H_\alpha(0))}\psi_2) &= \int \overline{\psi_1(x_1, \ldots, x_m, z_{m+1}, \ldots, z_{3N-3})}\, K(x, y) \\ &\quad \times \psi_2(y_1, \ldots, y_m, z_{m+1}, \ldots, z_{3N-3})\, d^m x\, d^m y\, d^{3N-3-m} z\end{aligned}$$

with

$$K(x, y) = (-1)^\sigma t^{-m/2} (2\pi i)^{-m/2} \prod_{i=1}^m |a_i|^{-1/2} \exp(i|x_i - y_i|^2/4a_i t)$$

where σ depends on the number of negative a_i.

Because of the $t^{-m/2}$ factor, $(\psi_1, e^{-it(H_\beta(0) - H_\alpha(0))}\psi_2) \to 0$ as $t \to \infty$. By an $\varepsilon/3$ argument, $(\psi_1, e^{-it(H_\beta(0) - H_\alpha(0))}\psi_2) \to 0$ for all ψ_1, ψ_2 and in particular $(\mathscr{T}_\alpha \varphi_\alpha, e^{-it(H_\beta(0) - H_\alpha(0))}\mathscr{T}_\beta \varphi_\beta) \to 0$. This proves the orthogonality of channels.

(c) Let $\psi \in \mathscr{H}_{\text{asym}}$. Then $\Omega^\pm \psi = \sum_\alpha \Omega_\alpha^\pm \psi_\alpha$. Since the $\Omega_\alpha^\pm \psi_\alpha$ are orthogonal to one another,

$$\|\Omega^\pm \psi\|^2 = \sum_\alpha \|\Omega_\alpha^\pm \psi_\alpha\|^2 = \sum_\alpha \|\Omega_{D(\alpha)}^\pm \mathscr{T}_\alpha \psi_\alpha\|^2 = \sum \|\psi_\alpha\|^2 = \|\psi\|^2$$

where we have used the fact that each $\mathscr{T}_\alpha$ and each $\Omega_\alpha^\pm$ is isometric.

(d) and (e) are proven as is the two-body case. ▮

Notice that $\mathscr{T}$ is not an isometry, for the Ran $\mathscr{T}_\alpha$ are not orthogonal to one another. For example, Ran $\mathscr{T}_\alpha = \mathscr{H}$ if α is the unique channel with $D(\alpha) = \{\{1\}, \ldots, \{N\}\}$. The proof that $\Omega^\pm$ are isometric depended critically on the fact that Ran $\Omega_\alpha^\pm$ are orthogonal to Ran $\Omega_\beta^\pm$ if $\alpha \neq \beta$. This in turn was essentially a consequence of the fact that $\lim_{t \to \pm\infty} \|\mathscr{T} e^{-itH_{\text{asym}}}\psi\| = \|\psi\|$ for all ψ, which was proven in (b) above.

We now define the S-operator:

Definition Let $S: \mathscr{H}_{\text{asym}} \to \mathscr{H}_{\text{asym}}$ be the operator $S = (\Omega^-)^*\Omega^+$. S is called the **S-operator, S-matrix,** or scattering operator. We also define $S_{\alpha\beta}: \mathscr{H}_\beta \to \mathscr{H}_\alpha$ by $S_{\alpha\beta} = (\Omega_\alpha^-)^*\Omega_\beta^+$ so that $S = \sum_{\alpha,\beta} S_{\alpha\beta}$.

For example, let $N = 3$, suppose that β is the unique channel with $D(\beta) = \{\{1\}, \{2\}, \{3\}\}$ and that α is a channel with $D(\alpha) = \{\{1, 2\}, \{3\}\}$. Then $S_{\alpha\beta}$ describes a capture process and $S_{\beta\alpha}$ describes a breakup.

As usual,

Definition If $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^- = \mathscr{H}_{\mathrm{ac}}(H)$, we say that the scattering for the N-body system is **complete**.

By rather involved methods, the following has been proven:

Theorem XI.37 Let $N = 3$, $\tilde{H} = \sum_{i=1}^{3} (-2m_i)^{-1}\Delta_i + \sum_{1\le i<j\le 3} V_{ij}$. Suppose that:

(i) Each V_{ij} obeys $V_{ij} \in L^{\frac{3}{2}+\varepsilon}(\mathbb{R}^3) \cap L^{\frac{3}{2}-\varepsilon}(\mathbb{R}^3)$ and $(1 + |x|)^{2+\varepsilon}V_{ij} \in L^2 + L^\infty$. (Roughly speaking, $V_{ij}(x)$ is required to have $|x|^{-2-\varepsilon}$ falloff.)

(ii) No two-body subsystem has a "zero energy resonance or bound state" in the following exact sense: Let $\mu_{ij} = (m_i^{-1} + m_j^{-1})^{-1}$. Let $k_{ij}(\lambda) = -(2\mu_{ij})^{-1}\Delta + \lambda V_{ij}(x)$ on $L^2(\mathbb{R}^3)$. Then the dimension of the spectral projection onto $(-\infty, 0)$ for $k_{ij}(\lambda)$ is independent of λ for $|\lambda - 1| < \delta$ for some $\delta > 0$. Moreover, no $k_{ij}(1)$ has a positive eigenvalue.

Then $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^- = \mathscr{H}_{\mathrm{ac}}(H)$.

For certain N-body systems with only one channel (that is, systems with no bound states for the $H(C)$), completeness has been proven; see Theorem XIII.27 for the case of weak coupling and Theorem XIII.32 for the case of repulsive potentials.

It seems likely that the methods of Section 17 will be extended to prove fairly strong results on asymptotic completeness for multiparticle Hamiltonians.

There is a final topic in the scattering of N-body systems which we would like to discuss, namely cluster properties of $\Omega^\pm$ and the related definition of the "connected part" of the S-matrix. These properties play a major role in further developments of N-body scattering, particularly in the physics literature. However, we caution the reader that the technical details are quite complicated and may be omitted since we shall not use these properties again. Cluster properties are simpler to express if we do not remove the center of mass motion. Thus let us define

$$\tilde{\mathscr{H}} = L^2(\mathbb{R}^3) \otimes \mathscr{H}, \qquad \tilde{\mathscr{H}}_{\mathrm{asym}} = L^2(\mathbb{R}^3) \otimes \mathscr{H}_{\mathrm{asym}}$$

$$\tilde{\Omega}_D^\pm = 1 \otimes \Omega_D^\pm, \qquad \tilde{\Omega}_\alpha^\pm = 1 \otimes \Omega_\alpha^\pm, \qquad \tilde{S} = 1 \otimes S, \qquad \tilde{\mathscr{T}}_\alpha = 1 \otimes \mathscr{T}_\alpha$$

$$\tilde{H} = h_0^{\mathrm{CM}} \otimes 1 + 1 \otimes H, \qquad \tilde{H}_{\mathrm{asym}} = h_0^{\mathrm{CM}} \otimes 1 + 1 \otimes H_{\mathrm{asym}}$$

Let i be in $\{1, \ldots, N\}$, $\mathbf{a}$ be in $\mathbb{R}^3$, and define $U^i(\mathbf{a})$ on $\tilde{\mathscr{H}}$ by:

$$(U^i(\mathbf{a})f)(\mathbf{x}_1, \ldots, \mathbf{x}_n) = f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_i - \mathbf{a}, \ldots, \mathbf{x}_n)$$

Given a cluster decomposition $D = \{C_1, \ldots, C_k\}$ and $\mathbf{a}_1, \ldots, \mathbf{a}_k \in \mathbb{R}^3$ we define $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ on $\tilde{\mathcal{H}}$ by

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \left(\prod_{i \in C_1} U^i(\mathbf{a}_1)\right)\left(\prod_{i \in C_2} U^i(\mathbf{a}_2)\right) \cdots \left(\prod_{i \in C_k} U^i(\mathbf{a}_k)\right)$$

Thus $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ translates the clusters relative to one another. To state the major technical result, which we shall then interpret, we need some other notions:

Definition Let $D^{(1)}$ and $D^{(2)}$ be two cluster decompositions. We say $D^{(2)}$ is a **refinement** of $D^{(1)}$ and write $D^{(1)} \lhd D^{(2)}$ if each element $C_\ell^{(2)}$ of $D^{(2)}$ is a subset of some $C_j^{(1)}$ of $D^{(1)}$.

Thus D_2 is a refinement of D_1 if each cluster in D_1 is obtained by grouping together one or more clusters in D_2. We write $D_1 \lhd D_2$ to indicate that several sets in D_2 are joined to form the sets in D_1.

If D is a cluster decomposition, there is associated a natural tensor product decomposition of $\tilde{\mathcal{H}}$ into $\otimes_{\ell=1}^{k} \tilde{\mathcal{H}}_{C_\ell}$ where $\tilde{\mathcal{H}}_{C_\ell}$ is the space of functions of the coordinates $\{\mathbf{r}_i \mid i \in C_\ell\}$. Suppose $D \lhd D'$. Then for each $C_\ell \in D$, D' induces a cluster decomposition D'_ℓ of C_ℓ by taking the family of elements of D' contained in C_ℓ. In such a case we write $\tilde{\Omega}^{\pm}_{D'_\ell}$ as the cluster channel wave operator on $\tilde{\mathcal{H}}(C_\ell)$ associated with the cluster D'_ℓ. Thus,

$$\tilde{\Omega}^{\pm}_{D'_\ell} = \operatorname*{s-lim}_{t \to \mp\infty} \exp(it\tilde{H}(C_\ell)) \exp\left(-it \sum_{C_j' \subset C_\ell} \tilde{H}(C_j')\right)$$

Theorem XI.38 Let $V_{ij} \in L^2(\mathbb{R}^3) + L^r(\mathbb{R}^3)$, $2 < r < 3$,

(a) If $D < D'$, then

$$\operatorname*{s-lim}_{\min_{i \neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)^{-1} \tilde{\Omega}^{\pm}_{D'} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell}$$

(b) If $D \lhd D'$, then

$$\operatorname*{s-lim}_{\min_{i \neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)^{-1} (\tilde{\Omega}^{\pm}_{D'})^* U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = \bigotimes_{\ell=1}^{k} (\tilde{\Omega}^{\pm}_{D'_\ell})^*$$

(c) If $D \not\lhd D'$ and β is any channel with $D(\beta) = D'$, then

$$\operatorname*{s-lim}_{\min_{i \neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty} (\tilde{\Omega}^{\pm}_{\beta})^* U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

Proof The proof of (a) is essentially identical to the proof of Theorem XI.33, so we sketch the major ideas leaving the details to the reader (Problem 54). One first notes that

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell} = \bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell}\, U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$

since $\prod_{i \in \mathscr{C}_\ell} U^i(\mathbf{a}_\ell)$ commutes with $\tilde{\Omega}^{\pm}_{D'_\ell}$, and that

$$\bigotimes_{i=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell} = \operatorname*{s-lim}_{t \to \mp\infty} e^{+i\tilde{H}_D t} e^{-i\tilde{H}_{D'} t}$$

Thus

$$\tilde{\Omega}^{\pm}_{D'} = \left(\operatorname*{s-lim}_{t \to \mp\infty} e^{+i\tilde{H} t} e^{-i\tilde{H}_D t}\right) \left[\bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell}\right] = \tilde{\Omega}^{\pm}_{D} \left[\bigotimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell}\right]$$

so to prove that $U_D^{-1}(\tilde{\Omega}^{\pm}_{D'} - \otimes_{\ell=1}^{k} \tilde{\Omega}^{\pm}_{D'_\ell})U_D$ goes strongly to 0, we need only prove that

$$\operatorname*{s-lim}_{\min_{i \neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty} U_D^{-1}(\mathbf{a})[\tilde{\Omega}^{\pm}_{D} - 1]U_D(\mathbf{a}) = 0 \tag{75}$$

But, for $\varphi \in D(H_0)$,

$$(\tilde{\Omega}^{\pm}_{D} - 1)\varphi = i \int_0^{\mp\infty} (e^{+i\tilde{H} t} I_D\, e^{-i\tilde{H}_D t} \varphi)\, dt$$

One proceeds now as we did in Theorem XI.33, using the estimates in Theorem XI.34 in place of those in Theorem XI.24. We defer the proof of (b) until after we prove (c).

(c) The heuristics behind this are that $(\Omega^{\pm}_{\beta})^*$ is zero on those states that asymptotically fail to form bound clusters in D'. Since $D \not\supset D'$, there is some pair $\langle i, j \rangle$ with $iD'j$ but $\sim iDj$. Thus $U_D(\mathbf{a})$ pries apart some cluster in D' as $\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty$ and prevents $U_D\psi$ from being a state that forms bound clusters in D'. This heuristic argument really has two elements; first U_D "pries apart clusters in D'," so we shall show that

$$\operatorname*{s-lim}_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} \mathscr{T}^*_{\beta} U_D(\mathbf{a}) = 0 \tag{76}$$

Secondly, $e^{-iHt}U_D(\mathbf{a})$ approaches $e^{-iH_D t}U_D(\mathbf{a})$ strongly as $\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty$; that is, as the clusters in D are moved apart, the part of the dynamics due to forces between the clusters becomes negligible.

As usual, to prove (76) it is enough to show that $\mathscr{T}^*_{\beta} U_D(a)\psi \to 0$ for a set of ψ whose linear combinations are dense in $\mathscr{H}$. Let $D' = \{C'_1, \ldots, C'_{k'}\}$ and pick $\psi = \varphi_1 \cdots \varphi_{k'}$ where φ_i is a function of the coordinates in C_i'. For each j, let $i(j)$ be that number so that $j \in C_i'$, one of the clusters of D. Suppose that

$$\beta = \begin{pmatrix} C_1' & \cdots & C_{k'}' \\ \eta_1 & \cdots & \eta_{k'}' \end{pmatrix}$$

Thus,

$$\|\mathscr{T}_\beta^* U_D(a)\psi\|_{\tilde{H}_\beta} = \prod_{\ell=1}^{k'} \left\| \int \eta_\ell(\xi^{(C_{\ell'})})\varphi(\{r_i + a_{i(j)}\}_{j \in C_{\ell'}})\, d\xi^{(C_\ell')} \right\|_{\tilde{H}(C_\ell')}$$

The point is that in some C_ℓ', there are j_1, j_2 with $i(j_1) \neq i(j_2)$. Thus, when the coordinates $\mathbf{r}_j + \mathbf{a}_{i(j)}$ in φ_ℓ are changed to $\mathbf{R}_\ell$, $\xi^{(C_\ell')}$ coordinates, some ξ's are translated as well as $\mathbf{R}_\ell$. Since we are taking an inner product in ξ with a fixed η, the norm $\| \cdots \|_{\tilde{H}(C_\ell')}$ will go to zero, so (76) is proven.

Next we prove that

$$\operatorname*{s-lim}_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} (e^{-i\tilde{H}t} - e^{-i\tilde{H}_D t})U_D(\mathbf{a}) = 0 \tag{77a}$$

and

$$\operatorname*{s-lim}_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} (e^{+i\tilde{H}_{D'}t} - e^{+i\tilde{H}_{D' * D}t})U_D(\mathbf{a})e^{-i\tilde{H}_D t} = 0 \tag{77b}$$

uniformly in t where $D' * D$ is the cluster decomposition whose elements are $\{C_\ell' \cap C_m\}$ when $1 \leq \ell \leq k'$, $1 \leq m \leq k$. This is just an expression of the fact that if we apply $U_D(\mathbf{a})$ to a vector ψ, thereby prying the clusters in D apart, interactions between clusters make negligible contributions to the dynamics. If $\psi \in D(\tilde{H}_0)$, then

$$(e^{-i\tilde{H}t} - e^{-i\tilde{H}_D t})U_D\psi = -ie^{-i\tilde{H}t} \int_0^t e^{+i\tilde{H}s} I_D e^{-i\tilde{H}_D s} U_D \psi\, ds$$

Thus to prove (77a) it is sufficient to prove that

$$\lim_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} \int_0^t \|I_D e^{-i\tilde{H}_D s} U_D(\mathbf{a})\psi\|\, ds = 0$$

uniformly in t. This is precisely the estimate we used in proving (75). To prove (77b), we need to prove that

$$\lim_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} \int_0^t \|(I_{D'} - I_{D * D'})e^{iH_{D * D'}s} U_D(\mathbf{a}) e^{-i\tilde{H}_0 s}\psi\|\, ds = 0$$

uniformly in t, and this is proven in a similar way (Problem 55).

Now we can put (76) and (77) together to obtain the desired result. From (77) and the relations

$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)e^{-i\mathcal{H}_0 t} = e^{-i\mathcal{H}_0 t}U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$
$$U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)e^{-i\mathcal{H}_{D * D'} t} = e^{-i\mathcal{H}_{D * D'} t}U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$$

one obtains that for any $\psi \in \mathscr{H}$,

$$\sup_{t \in \mathbb{R}} \|(e^{i\mathcal{H}_{D'} t}e^{-i\mathcal{H} t} - e^{i\mathcal{H}_{D * D'} t}e^{-i\mathcal{H}_D t})U_D\psi\| \to 0 \tag{78}$$

as $\min_{i \neq j}|\mathbf{a}_i - \mathbf{a}_j| \to \infty$. Let $\tilde{\Omega}^{\pm}_{D;\, D * D'} = \text{s-lim}_{t \to \mp\infty}\, e^{i\mathcal{H}_D t}e^{-i\mathcal{H}_{D * D'} t}$ which exists by Theorem XI.34. Then

$$(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}_{D;\, D * D'})^* U_D(\mathbf{a})\psi = \underset{t \to \mp\infty}{\text{w-lim}}\, (e^{i\mathcal{H}_{D'} t}e^{-it\mathcal{H}} - e^{i\mathcal{H}_{D' * D} t}e^{-i\mathcal{H}_D t})U_D(\mathbf{a})\psi$$

for each fixed ψ and $\mathbf{a}$. From the fact that $\|\text{w-lim}_{t \to \pm\infty}\, \psi_t\| \leq \lim_{t \to \pm\infty} \|\psi_t\|$, and (78) it follows that

$$\lim_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} \|(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}^{\pm}_{D,\, D * D'})^* U_D(a)\psi\| = 0$$

Finally, since $(\tilde{\Omega}^{\pm}_{D,\, D * D'})^* U_D(\mathbf{a}) = U_D(\mathbf{a})(\tilde{\Omega}^{\pm}_{D,\, D * D'})^*$, we conclude

$$\begin{aligned} \underset{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty}{\text{s-lim}} \mathscr{T}^*_\beta(\tilde{\Omega}^{\pm}_{D'})^* U_D(\mathbf{a}) &= \underset{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty}{\text{s-lim}} \mathscr{T}^*_\beta U_D(\mathbf{a})(\tilde{\Omega}^{\pm}_{D;\, D * D'})^* \\ &= 0 \end{aligned}$$

This proves (c).

(77) holds whether $D \lhd D'$ or not, so its consequence s-lim $\|(\tilde{\Omega}^{\pm}_{D'} - \tilde{\Omega}^{\pm}_{D,\, D * D'})^* U_D(\mathbf{a})\psi\| = 0$ holds. If $D \lhd D'$, then $D * D' = D'$ and $\tilde{\Omega}^{\pm}_{D,\, D * D'} = \bigotimes_{\ell=1}^k \Omega^{\pm}_{D_\ell}$. This fact and $U_D^{-1}(\bigotimes_{\ell=1}^k \tilde{\Omega}^{\pm}_{D_\ell})^* U_D = (\bigotimes_{\ell=1}^k \tilde{\Omega}^{\pm}_{D_\ell})^*$ imply the result in (b). ▌

Now we use these cluster properties to obtain information about the S-operator. Let α be a channel and D a cluster decomposition with $D \lhd D(\alpha)$. In D some of the bound fragments in channel α are clumped together. This clumping induces a breakup of α into *subchannels*; namely, for each $C_\ell \in D$, let α_ℓ be the collection of clusters $F_m \in D(\alpha)$ with $F_m \subset C_\ell$ together with the bound states η_m in α. Thus, if $D = \{\{1, 2\}, \{3, 4, 5\}, \{6\}\}$ and

$$\alpha = \begin{pmatrix} \{1\} & \{2\} & \{3, 4\} & \{5\} & \{6\} \\ 1 & 1 & \varphi(\mathbf{r}_{34}) & 1 & 1 \end{pmatrix}$$

where $\varphi(\mathbf{r}_{34})$ is some bound state of $H(\{3, 4\})$, then

$$\alpha_1 = \begin{pmatrix} \{1\} & \{2\} \\ 1 & 1 \end{pmatrix}, \qquad \alpha_2 = \begin{pmatrix} \{3, 4\} & \{5\} \\ \varphi(\mathbf{r}_{34}) & 1 \end{pmatrix}, \qquad \alpha_3 = \begin{pmatrix} \{6\} \\ 1 \end{pmatrix}$$

The collection $\{\alpha_\ell\}_{\ell=1}^k$ is called the **decomposition of α induced by D**. Let $D = \{C_1, \ldots, C_k\}$ and let α, β be channels with $D \triangleleft D(\beta)$, $D \triangleleft D(\alpha)$. Let $\{\alpha_\ell\}_{\ell=1}^k$ and $\{\beta_\ell\}_{\ell=1}^k$ be the decompositions of α and β induced by D. Then we shall write $S_{\alpha_\ell, \beta_\ell}^{(C_\ell)}$ for the S-operator for the n_ℓ-body system which describes scattering from α_ℓ to β_ℓ.

Now let $D \triangleleft D(\alpha)$. Then $U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ leaves Ran $\tilde{\mathscr{F}}_\alpha$ invariant and so induces a map $U_D^{(\alpha)}(\mathbf{a}_1, \ldots, \mathbf{a}_k)$ on $\tilde{\mathscr{H}}_\alpha$ by $U_D \tilde{\mathscr{F}}_\alpha = \tilde{\mathscr{F}}_\alpha U_D^{(\alpha)}$. Specifically, if $\varphi \in \tilde{\mathscr{H}}_\alpha$ is a function of $\langle \mathbf{r}_{F_1}, \ldots, \mathbf{r}_{F_m} \rangle$ where $D(\alpha) = \{F_1, \ldots, F_m\}$, then $U_D^{(\alpha)}$ acts on $\tilde{\mathscr{H}}_\alpha$ by translating those F_m in C_ℓ by $\mathbf{a}_\ell$. Fix $\psi \in \tilde{\mathscr{H}}_\alpha$ and consider the states $U_D^{(\alpha)}(\mathbf{a}_1, \ldots, \mathbf{a}_k)\psi$ as $\min_{i \neq j} |\mathbf{a}_i - \mathbf{a}_j| \to \infty$. How do we expect $\tilde{S} U_D^\alpha \psi$ to behave? Let β be a channel with $D \ntriangleleft D(\beta)$. Then to scatter into β from α, particles in different clusters $C_\ell \in D$ must come together. Since the clusters in D are far apart in $U_D^\alpha \psi$, we expect no scattering into β. On the other hand, if $D \triangleleft D(\beta)$, one can scatter into β by scattering separately into each $C_\ell \in D$. We expect $\tilde{S} U_D^{(\alpha)} \psi$ to factor into separate scattering for each cluster C_ℓ. This is in fact true.

Theorem XI.39 (spatial cluster properties of S) Let α be a channel of an N-body quantum system that obeys the hypotheses of Theorem XI.34. Let D be a cluster decomposition with $D \triangleleft D(\alpha)$.

(a) If $D \triangleleft D(\beta)$, then

$$\operatorname*{s-lim}_{\min_{i \neq j} |\mathbf{a}_i - \mathbf{a}_j| \to \infty} \left(\tilde{S}_{\beta\alpha} - \bigotimes_{\ell=1}^k \tilde{S}_{\beta_\ell \alpha_\ell}^{(C_\ell)} \right) U_D^{(\alpha)}(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

(b) If $D \ntriangleleft D(\beta)$, then

$$\operatorname*{s-lim}_{\min_{i \neq j} |\mathbf{a}_i - \mathbf{a}_j| \to \infty} \tilde{S}_{\beta\alpha} U_D^{(\alpha)}(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0$$

Proof To prove (a), we use Theorem XI.38a and b to first see that

$$\text{s-lim} \left(\tilde{S}_{\beta\alpha} U_D^{(\alpha)} - \tilde{\mathscr{F}}_\beta^* U_D \bigotimes_{\ell=1}^k \tilde{\Omega}_{D(\beta_\ell)}^- \tilde{\Omega}_{\alpha_\ell}^+ \right) = 0$$

for

$$\tilde{S}_{\beta\alpha} U_D^{(\alpha)} - (\tilde{\Omega}_\beta^-)^* \left[U_D \bigotimes_{\ell=1}^k \tilde{\Omega}_{\alpha_\ell}^+ \right] = (\tilde{\Omega}_\beta^-)^* \left[\tilde{\Omega}_\alpha^+ U_D^{(\alpha)} - U_D \bigotimes_{\ell=1}^k \tilde{\Omega}_{\alpha_\ell}^+ \right]$$

goes to zero strongly by Theorem XI.38a and similarly,

$$\begin{aligned}(\Omega_\beta^-)^*\left[U_D \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{\alpha_\ell}^+\right] - \mathscr{T}_\beta^* U_D \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{D(\beta_\ell)}^- \tilde{\Omega}_{\alpha_\ell}^+ \\ = \mathscr{T}_\beta^*\left[(\tilde{\Omega}_{D(\beta)}^-)^* U_D - U_D \bigotimes_{\ell=1}^{k} (\tilde{\Omega}_{D(\beta)}^-)^*\right] \bigotimes_{\ell=1}^{k} \tilde{\Omega}_{\alpha_\ell}^+\end{aligned}$$

goes to zero strongly by Theorem XI.38b. Finally, we remark that

$$\left(\bigotimes_{\ell=1}^{k} \mathscr{T}_{\beta_\ell}^* \tilde{\Omega}_{D(\beta_\ell)}^- \tilde{\Omega}_{\alpha_\ell}^+\right) U_D^{(\alpha)} = \bigotimes_{\ell=1}^{k} \tilde{S}_{\beta_\ell \alpha_\ell}^{(C_\ell)} U_D^{(\alpha)}$$

To prove (b), we use Theorem XI.38c in place of Theorem XI.38b. ▌

Corollary If the S-matrix of an N-body quantum system obeying the hypotheses of Theorem XI.34 is unitary, then the S-matrix of any subsystem is unitary.

These spatial cluster properties are interesting because of their direct physical interpretation, but they are more important because of the "p-space smoothness" which they suggest. To understand the phenomenon which we are discussing, let us first consider two-body scattering. The $\tilde{S}$-operator is given by a kernel. One way of seeing this is to note that if $\varphi, \psi \in \mathscr{S}(\mathbb{R}^6)$, then $\langle \bar{\varphi}, \psi \rangle \to (\varphi, \tilde{S}\psi)$ is bilinear and continuous on $\mathscr{S}$ so there is a distribution $Q(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_3, \mathbf{x}_4)$ in $\mathscr{S}'(\mathbb{R}^{12})$ with

$$(\varphi, \tilde{S}\psi) = \int \overline{\varphi(\mathbf{x}_1, \mathbf{x}_2)} Q(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_3, \mathbf{x}_4) \psi(\mathbf{x}_3, \mathbf{x}_4)\, d^3x_1 \cdots d^3x_4$$

It is useful to write $\tilde{S}$ in p-space, that is, to look at the kernel of $\mathscr{F}\tilde{S}\mathscr{F}^{-1}$ where $\mathscr{F}$ is the Fourier transform:

$$(\varphi, \tilde{S}\psi) = \int \overline{\hat{\varphi}(p_1, p_2)} s(p_1, p_2; p_3, p_4) \hat{\psi}(p_3, p_4)\, d^3p_1 \cdots d^3p_4$$

Because of conservation of energy and momentum, that is, because S commutes with space translations and the *free* dynamics, the distribution s has support on the manifold where

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4$$

$$E_{\text{out}} \equiv \frac{\mathbf{p}_1^2}{2\mu_1} + \frac{\mathbf{p}_2^2}{2\mu_2} = \frac{\mathbf{p}_3^2}{2\mu_3} + \frac{\mathbf{p}_4^2}{2\mu_4} \equiv E_{\text{in}}$$

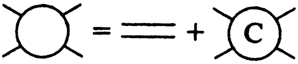
This suggests that s may be written in the form:

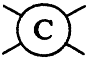
$$s(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4) = \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)\delta(E_{\text{in}} - E_{\text{out}}) s^{\text{red}}(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4)$$

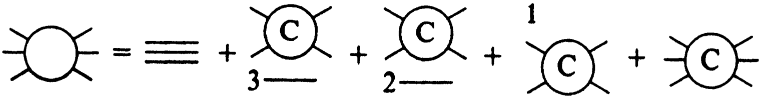
A priori, s could have much more complicated singularities such as $-\Delta\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)$. That such a δ-function singularity factors out is something we shall see when we discuss the reduction of the S-matrix by symmetries in Section 8. One might hope that s^{red} is a smooth function of the variables $\mathbf{p}_1, \ldots, \mathbf{p}_4$ as long as we vary them on the manifold where energy and momentum are conserved. This is not a good conjecture however! For let $U(\mathbf{a})$ be translation of the first particle by $\mathbf{a}$. Then $U(\mathbf{a})\tilde{S}U(\mathbf{a})^{-1}$ has a kernel $se^{i\mathbf{a}\cdot(\mathbf{p}_1 - \mathbf{p}_3)}$. If s^{red} were smooth, the Riemann–Lebesgue lemma would imply that $\lim_{\mathbf{a}\to\infty} (\varphi, U(\mathbf{a})\tilde{S}U(\mathbf{a})^{-1}\psi) = 0$, but we know that $\lim_{\mathbf{a}\to\infty} (\varphi, U(\mathbf{a})(\tilde{S} - I)U(\mathbf{a})^{-1}\psi) = 0$. This suggests that $\tilde{S} - I$ should have a smooth kernel; that is, we hope that

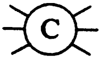
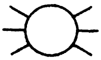
$$\begin{aligned} s(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4) &= \delta(\mathbf{p}_1 - \mathbf{p}_3)\delta(\mathbf{p}_2 - \mathbf{p}_4) \\ &\quad - (2\pi i)\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3 - \mathbf{p}_4)\delta(E_{\text{in}} - E_{\text{out}})t(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p}_3, \mathbf{p}_4) \end{aligned}$$

where t is a smooth function of $\mathbf{p}_i$ if we vary $\langle \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4 \rangle$ staying on the manifold where momentum and energy are conserved. The $\delta(\mathbf{p}_1 - \mathbf{p}_2)\delta(\mathbf{p}_3 - \mathbf{p}_4)$ term is just the kernel of the operator I. We put in the $2\pi i$ factor for conventional reasons. In the two-body case, we shall actually prove that s has this form for a wide variety of potentials; see Sections 6 and 7. What can we expect in the N-body case? Write the two-body result schematically



where  stands for the part with a smooth kernel; this part is called the "connected" part. One might guess for the three-body case:



so we can define  recursively in terms of  and the connected parts for fewer particles.

Definition Let α, β be channels of an N-body system. Define $R_{\alpha\beta}$ recursively (in N) by

$$R_{\alpha\beta} = \tilde{S}_{\alpha\beta} - \sum_{D \in \mathscr{C}_{\alpha\beta}} R_{\alpha_1\beta_1} \cdots R_{\alpha_k\beta_k}$$

where $\mathscr{C}_{\alpha,\beta}$ is the set of cluster decompositions with $D \lhd D(\alpha)$, $D \lhd D(\beta)$ *for which D contains at least two clusters.* For $N = 2$, $R = S - I$.

The spatial cluster properties of Theorem XI.39 then imply (Problem 56):

Theorem XI.40 (spatial cluster property of the reduced S-operators)

(a) $$\tilde{S}_{\alpha\beta} = \sum_{\substack{D \lhd D(\alpha),\, D \lhd D(\beta) \\ D = \{C_1, \ldots, C_k\}}} R_{\alpha_1\beta_1} R_{\alpha_2\beta_2} \cdots R_{\alpha_k\beta_k}$$

(b) $$\operatorname*{s-lim}_{\min_{i \neq j}|a_i - a_j| \to \infty} R_{\alpha\beta} U_D(\mathbf{a}_1, \ldots, \mathbf{a}_k) = 0 \qquad \text{for all } D$$

with $D \lhd D(\beta)$.

This *suggests* that $R_{\alpha\beta}$ has a kernel of the form

$$r_{\alpha\beta}(\mathbf{p}, \mathbf{p}') = (2\pi i)\, \delta\left(\sum_{i=1}^{N} \mathbf{p}_i - \sum_{i=1}^{N} \mathbf{p}_i'\right) \delta(E - E') t_{\alpha\beta}(\mathbf{p}, \mathbf{p}')$$

where $t_{\alpha\beta}$ is a smooth function of $\mathbf{p}, \mathbf{p}'$. In fact, the "hypothesis of the analytic S-matrix" demands that $t_{\alpha\beta}(\mathbf{p}, \mathbf{p}')$ be the boundary value of a function analytic in certain regions. Unfortunately, this attractive hypothesis has not been proven in many-channel, many-body systems. In the Notes we shall discuss those results that constitute a partial proof of the "hypothesis of the analytic S-matrix" for quantum systems with $N \geq 3$.

XI.6 Quantum scattering III: Eigenfunction expansions

Any formal manipulations that are not obviously wrong are assumed to be correct.

M. L. Goldberger and K. Watson in **Scattering Theory**

For two-body quantum systems with potentials having $|x|^{-1-\varepsilon}$ falloff as $|x| \to \infty$, we have established the existence and uniqueness of scattering states. Completeness will be proven in Sections 17 and XIII.8. We have not, however, discussed any way of explicitly "computing" the S-operator or of correlating experimental data with the theory. Our goal in this section is to establish certain formulas which normally go under the name "formal scattering theory" or "time-independent scattering theory." These formulas present the S-operator as an explicit "integral operator" with kernel

$\delta(\mathbf{k}-\mathbf{k}') - 2\pi i\,\delta(k^2 - k'^2)T(\mathbf{k}, \mathbf{k}')$; see Theorem XI.42. In the next section we shall prove that the function $T(\mathbf{k}, \mathbf{k}')$ has an analytic continuation into certain regions.

The main tool in "formal scattering theory" is an eigenfunction expansion for the Hamiltonian H which is of considerable interest for its own sake. An operator A on $L^2(\mathbb{R}^3, dx)$ with purely discrete spectrum has an eigenfunction expansion in the direct sense that there are L^2 functions $\varphi_n(x)$ with an associated map $\tilde{}: L^2(\mathbb{R}^3, dx) \to \ell_2$ by

$$(\tilde{f})_n = \int \overline{\varphi_n(x)} f(x)\, dx \tag{79a}$$

That the φ_n are eigenfunctions with $A\varphi_n = a_n \varphi_n$ can be expressed by

$$(\widetilde{Af})_n = a_n \tilde{f}_n \qquad \text{if } f \in D(A) \tag{79b}$$

The orthonormality of the $\{\varphi_n\}$ implies

$$\text{Ran}\ \tilde{} = \ell_2 \tag{79c}$$

The completeness of the φ_n is expressed by

$$f(x) = L^2\text{-lim} \sum_{n=0}^{\infty} \tilde{f}_n \varphi_n(x) \tag{79d}$$

Finally, as a consequence of completeness and orthonormality:

$$\|f\|^2 = \sum_n |\tilde{f}_n|^2 \tag{79e}$$

Two-body Hamiltonians with center of mass removed have lots of spectrum that is nondiscrete—in fact, there is absolutely continuous spectrum $[0, \infty)$ associated with scattering. However, we can hope that some sort of "continuum" eigenfunction expansion exists. As a model of what we are seeking, we shall show how the Fourier transform provides an eigenfunction expansion for $H_0 = -\Delta$ which has only continuous spectrum. Write $\varphi_0(x, k) = e^{ik\cdot x}$ and think of $\varphi_0(\cdot, k)$ as a family of functions of x parametrized by a continuous index k. Then, we know that $\hat{}$ satisfies

$$\hat{f}(k) = (2\pi)^{-n/2}\ \text{l.i.m.} \int \overline{\varphi_0(x, k)} f(x)\, dx \tag{80a}$$

where $\text{l.i.m.} \int = L^2\text{-lim} \int_{|x|<M}$ as $M \to \infty$. The $\varphi_0(\cdot, k)$ are eigenfunctions with eigenvalue k^2 in the sense that

$$(\widehat{H_0 f})(k) = k^2 \hat{f}(k) \qquad \text{if } f \in D(H_0) \tag{80b}$$

The orthogonality and "normalization" of the $\varphi_0(\cdot, k)$ imply

$$\operatorname{Ran} \,\hat{}\, = L^2(\mathbb{R}^3, dx) \tag{80c}$$

The completeness of the set $\{\varphi_0(\cdot, k)\}_{k \in \mathbb{R}^n}$ is expressed by

$$f(x) = \text{l.i.m.}\ (2\pi)^{-3/2} \int \varphi_0(x, k)\hat{f}(k)\, dk \tag{80d}$$

and

$$\|f\|^2 = \int |\hat{f}(k)|^2\, dk \tag{80e}$$

How can we find candidates φ for the "continuum eigenfunctions" needed for an eigenfunction expansion of $H = H_0 + V$? $\Omega^+ f$ has been defined only for $f \in L^2$, but suppose that we could make sense out of $\Omega^+\varphi_0(\cdot, k)$. Then, since $\Omega^+ H_0 = H\Omega^+$, $\varphi(\cdot, k) \equiv \Omega^+\varphi_0(\cdot, k)$ should obey $H\varphi = k^2\varphi$ in the sense of (80b). If $\varphi = \Omega^+\varphi_0$ in some sense, then $\varphi_0 = (\Omega^+)^*\varphi$ should be the limit as $t \to -\infty$ of

$$\begin{aligned} e^{+iH_0t}e^{-iHt}\varphi &= \varphi - i\int_0^t e^{iH_0s}Ve^{-iHs}\varphi\, ds \\ &\to \varphi - \lim_{\varepsilon \downarrow 0} i\int_0^{-\infty} e^{iH_0s}Ve^{-ik^2s}e^{+\varepsilon s}\varphi\, ds \\ &= \varphi + \lim_{\varepsilon \downarrow 0} (H_0 - k^2 - i\varepsilon)^{-1}V\varphi \end{aligned}$$

Thus φ should obey

$$\varphi(\cdot, k) = \varphi_0(\cdot, k) - \lim_{\varepsilon \downarrow 0} ([H_0 - (k^2 + i\varepsilon)]^{-1}V\varphi)(\cdot, k) \tag{81a}$$

or, using (IX.30),

$$\varphi(\mathbf{x}, \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\int \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, d\mathbf{y} \tag{81b}$$

Physicists call Ω^+ the wave operator as $t \to -\infty$ because of the $+i\varepsilon$ in (81a). (81), an equation that we arrived at by heuristic argument, is known as the **Lippmann–Schwinger equation**. To find candidates φ for an eigenfunction expansion, we shall solve this equation. Once we have φ, we shall form the eigenfunction transform $f^*(k) = \text{l.i.m.}(2\pi)^{-3/2} \int \overline{\varphi(x, k)} f(x)\, dx$. We expect analogues of (80) to hold with one exception: The $\varphi(\cdot, k)$ will not in general be complete; that is, we no longer expect

$$f(x) = \text{l.i.m.}(2\pi)^{-3/2} \int f^*(k)\varphi(x, k)\, dk$$

since the φ's are only eigenfunctions associated with the absolutely continuous spectrum of H. Indeed, we shall find that $(P_{ac}(H)f)(x) = \text{l.i.m.}(2\pi)^{-3/2} \int f^*(k)\varphi(x, k)\, dk$. Finally, we expect that this eigenfunction transform and the Fourier transform should be related; for formally $\Omega^+\varphi_0 = \varphi$, which suggests that $\Omega^+(\int b(k)\varphi_0(x, k)\, dk) = \int b(k)\varphi(x, k)\, dk$ or that $(\Omega^+ f)^* = \hat{f}$ where we let $\hat{f} = (2\pi)^{3/2} b$.

The main result of this section (Theorem XI.41) is that all of the above conjectures are correct. Recall that the Rollnik class R is the set of measurable functions $V(x)$ satisfying

$$\|V\|_R^2 = \int_{\mathbb{R}^6} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, dx\, dy < \infty$$

Theorem XI.41 Let V be in $R \cap L^1(\mathbb{R}^3)$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let $H = H_0 + V$ in the sense of quadratic forms (Theorem X.19). Then, there is a set $\mathscr{E} \subset \mathbb{R}_+$, the positive reals, which is closed, of Lebesgue measure zero, and such that:

(a) If $k^2 \notin \mathscr{E}$, then there is a unique solution $\varphi(\cdot, \mathbf{k})$ of the Lippmann–Schwinger equation (81) which obeys $|V|^{1/2}\varphi(\cdot, \mathbf{k}) \in L^2$.

(b) If $f \in L^2$, then

$$f^*(\mathbf{k}) = \text{l.i.m.}(2\pi)^{-3/2} \int \overline{\varphi(\mathbf{x}, \mathbf{k})} f(\mathbf{x})\, d\mathbf{x} \tag{82a}$$

exists.

(c) If $f \in D(H)$, then

$$(Hf)^*(\mathbf{k}) = k^2 f^*(\mathbf{k}) \tag{82b}$$

(d) Ran $^* = L^2(\mathbb{R}^3)$ and (82c)

$$\int |f^*(\mathbf{k})|^2\, d\mathbf{k} = \|P_{ac}(H)f\|^2 \tag{82e}$$

More generally, if $[\alpha, \beta] \cap \mathscr{E}$ is empty and $\alpha > 0$, then

$$\int_{\alpha \le k^2 \le \beta} |f^*(\mathbf{k})|^2\, dk = \|P_{[\alpha,\beta]}(H)f\|^2 \tag{82e$'$}$$

where $\{P_\Omega(H)\}$ is the spectral family for H.

(e) Let L.I.M. stand for the L^2-limit as $M \to \infty$ and $\delta \to 0$ of the integral over $\{\mathbf{k} \mid k \le M, \text{dist}(k^2, \mathscr{E}) > \delta\}$. Then

$$(P_{ac}(H)f)(x) = \text{L.I.M.}(2\pi)^{-3/2} \int f^*(\mathbf{k})\varphi(\mathbf{x}, \mathbf{k})\, d\mathbf{k} \tag{82d}$$

(f) For any $f \in L^2$,

$$(\Omega^+ f)^\#(\mathbf{k}) = \hat{f}(\mathbf{k}) \tag{83}$$

We shall sketch the major ideas in the proof of Theorem XI.41. The details may be found in the references in the Notes. But first we examine several consequences of the theorem and its proof. Notice first that (82e′) implies that for any interval $[\alpha, \beta]$, disjoint from $\mathscr{E}$ with $\alpha > 0$, $\operatorname{Ran} P_{[\alpha, \beta]} \subset \mathscr{H}_{\text{ac}}$; so if any singular continuous spectrum exists, it must be in $\mathscr{E}$ since $\sigma_{\text{ess}}(H) = [0, \infty)$ by Theorem XIII.15. This will allow us to conclude that $\sigma_{\text{sing}}(H) = \varnothing$ in some cases (see Theorem XIII.21). Secondly, in the proof of Theorem XI.41, one uses the fact that Ω^+ exists but not its completeness. (83) says that $\#[\operatorname{Ran} \Omega^+] = L^2$ and (82d) says that $\#^{-1}[L^2] = \mathscr{H}_{\text{ac}}$, so that Theorem XI.41 implies that $\operatorname{Ran} \Omega^+ = \mathscr{H}_{\text{ac}}$. Thus, in case $V \in L^1 \cap R$, we have a proof of the completeness of $\Omega^\pm$ which does not use the Kato–Birman theory. In the Notes we explain how the eigenfunction expansion helps to "explain" the convergence of the wave operators when $V_n \to V$ in R and L^1. In the Notes we shall also discuss how the method used to prove Theorem XI.41 can be used to prove a similar result when $V \in L^p \cap L^{3/2}$ for some $1 \le p < \frac{3}{2}$ (see also Problem 57). We shall discuss similar eigenfunction expansions in a more general setting in the appendix and in the Notes. We also remark that if $\sigma_{\text{sing}}(H) = \varnothing$ (see Sections XIII.6, 7, 8), we can find a family $\{\varphi_n\}_{n=1}^N$ of square integrable eigenfunctions for H with $H\varphi_n = E_n \varphi_n$ so that, if $f_n^\# = (\varphi_n, f)$, then

$$f(\mathbf{x}) = \text{L.I.M.}\left(\sum_{n=1}^{N} f_n^\# \varphi_n(\mathbf{x}) + \int (2\pi)^{-3/2} \varphi(\mathbf{x}, \mathbf{k}) f^\#(\mathbf{k}) \, d\mathbf{k} \right)$$

$$\|f\|^2 = \sum_{n=1}^{N} |f_n^\#|^2 + \int |f^\#(\mathbf{k})|^2 \, d\mathbf{k}$$

$$(Hf)^\#(\mathbf{k}) = k^2 f^\#(\mathbf{k}); \; (Hf)_n^\# = E_n f_n^\#$$

We now turn to the main ideas in the proof of Theorem XI.41:

(I) *Modified Lippmann–Schwinger equation* We first introduce a modified Lippmann–Schwinger equation. If $\psi(x, k) = |V(x)|^{1/2} \varphi(x, k)$ and φ obeys (81), then ψ obeys

$$\psi(x, k) = |V(x)|^{1/2} e^{ik \cdot x} - \frac{1}{4\pi} \int \frac{|V(x)|^{1/2} e^{i|k|\,|x-y|} V^{1/2}(y)}{|x - y|} \psi(y, k) \, dy \tag{84}$$

where $V^{1/2} = |V|^{1/2}(\operatorname{sgn} V)$.

We first show that (84) has solutions. Since $V \in L^1 \cap R$, $e^{ik\cdot x}|V|^{1/2}$ is in $L^2(\mathbb{R}^3)$ and

$$\frac{|V(x)|^{1/2}e^{i|k|\,|x-y|}V^{1/2}(y)}{|x-y|} \in L^2(\mathbb{R}^6)$$

for any k in $\mathbb{R}^3$. Thus the modified Lippmann–Schwinger equation has the form $\psi = \eta + L_{|k|}\psi$ where η is in L^2 and $L_{|k|}$ is a Hilbert–Schmidt operator. Let $\mathscr{E}$ be the set of $|k|^2 \in \mathbb{R}_+$ such that the homogeneous equation $\psi = L_{|k|}\psi$ has a nonzero solution in L^2. By the Fredholm alternative (corollary to Theorem VI.14), (84) has a unique L^2 solution ψ whenever $|k|^2 \notin \mathscr{E}$. It follows that the original Lippmann–Schwinger equation has a unique solution φ satisfying $|V|^{1/2}\varphi \in L^2(\mathbb{R}^3)$ given by

$$\varphi(x, k) = e^{ik\cdot x} - \frac{1}{4\pi}\int \frac{e^{i|k|\,|x-y|}}{|x-y|} V^{1/2}(y)\psi(y, k)\,dy$$

Of course, one must do a little arguing to show this last integral converges a.e. in x, but we are not giving the details of such subtleties in this sketch.

(II) *Study of the set* $\mathscr{E}$ Let K_λ be the operator $|V|^{1/2}(H_0 - \lambda^2)^{-1}V^{1/2}$. This is the integral operator (84) when $\lambda = |k|$ for some $k \in \mathbb{R}^3$, in particular, for real positive λ. K_λ is easily shown to be analytic when $\operatorname{Im}\lambda > 0$ and continuous when $\operatorname{Im}\lambda \geq 0$. Moreover, by the dominated convergence theorem, one can show that the Hilbert–Schmidt norm of K_λ goes to 0 as $\operatorname{Im}\lambda \to \infty$. Thus $(I + K_\lambda)^{-1}$ exists as long as $\operatorname{Im}\lambda$ is large. At this point we need a slight improvement of the analytic Fredholm theorem (Theorem VI.14), namely:

Proposition Let $A(\lambda)$ be a compact operator-valued function in $D = \{\lambda \mid \operatorname{Im}\lambda \geq 0\}$ which is continuous in D and analytic in its interior. Then either $(1 - A(\lambda))^{-1}$ exists for no λ in D or $\{\lambda \mid \operatorname{Im}\lambda = 0$, and $(1 - A(\lambda))^{-1}$ does not exist$\}$ is a closed subset of $\mathbb{R}$ with measure 0.

This proposition follows from the method of proof of Theorem VI.14 together with a fact about analytic functions: The real zeros of a function analytic in the open upper half-plane and continuous in the closed half-plane is a closed subset of $\mathbb{R}$ of measure 0 (see Problems 58 and 59 and the Notes). Thus the subset $\mathscr{E} \subset \mathbb{R}$ defined in part I is closed with measure 0.

We make several remarks about $\mathscr{E}$: First, $\mathscr{E}$ is always bounded. This follows from the fact that the operator norm of K_λ goes to zero as $\lambda \to \infty$, λ real, due to the oscillations of the kernel. These oscillations are controlled by the Riemann–Lebesgue lemma (Problem 60). Secondly, we note that there are two cases in which we have control on $\mathscr{E}$. If $\|V\|_R < 4\pi$, then $\|K_\lambda\| < 1$ for all λ so $\mathscr{E} = \varnothing$. Or, if V falls off exponentially in the sense that $e^{\alpha|x|}V(x) \in R$ for some $\alpha > 0$, then $\mathscr{E}$ is finite. This is because in that case K_λ can be continued to the region $\{\lambda \,|\, \text{Im}\,\lambda > -\alpha/2\}$ so that the ordinary analytic Fredholm theorem implies that $\mathscr{E}$ is discrete.

(III) *Study of the Green's function* The basic idea of the proof is to relate the functions $\varphi(x, k)$ to the integral operator $(H - E)^{-1}$ and then to relate $(H - E)^{-1}$ to the spectral projections via Stone's formula (Theorem VII.13),

$$\operatorname*{s-lim}_{\varepsilon \downarrow 0}(2\pi i)^{-1} \int_\alpha^\beta [(H - \mu - i\varepsilon)^{-1} - (H - \mu + i\varepsilon)^{-1}]\, d\mu = \tfrac{1}{2}P_{(\alpha,\beta)} + \tfrac{1}{2}P_{[\alpha,\beta]}$$

As a preliminary, it is necessary to study the integral kernel of $(H - E)^{-1}$.

Lemma 1 Suppose $E \notin \sigma(H)$. Then there exists a measurable function $G(x, y; E)$ on $\mathbb{R}^3 \times \mathbb{R}^3$, so that

$$[(H - E)^{-1}\psi](x) = \int G(x, y; E)\psi(y)\, dy$$

Moreover:

(a) For almost every fixed x, $G(x, \cdot\,; E) \in L^1 \cap L^2$.
(b) $G(x, y; E) = G(y, x; E)$ and $\overline{G(x, y; E)} = G(x, y; \bar{E})$.
(c) G obeys the integral equation

$$G(x, y; E) = G_0(x, y; E) - \int G_0(x, z; E)V(z)G(z, y; E)\, dz$$

where $G_0(x, y; E) = e^{i\sqrt{E}|x-y|}/4\pi|x - y|$ is the free Green's function where we take the value of $\sqrt{E}$ with the positive imaginary part.

Proof We present the formal elements of the proof, not worrying about convergence of integrals or domain questions. By a simple argument (Problem 61),

$$\begin{aligned}(H - E)^{-1} = (H_0 - E)^{-1} &- [(H_0 - E)^{-1}V^{1/2}] \\ &\times [1 + |V|^{1/2}(H_0 - E)^{-1}V^{1/2}]^{-1}[|V|^{1/2}(H_0 - E)^{-1}]\end{aligned}$$

Since $V \in L^1$, the kernel $|V(x)|^{1/2}e^{i\sqrt{E}|x-y|}/4\pi|x - y|$ of $|V|^{1/2}(H_0 - E)^{-1}$ is Hilbert–Schmidt. Thus $(H - E)^{-1} - (H_0 - E)^{-1}$ is Hilbert–Schmidt and so is an integral operator with a square integrable kernel $A(x, y)$. In particular, $A(x, \cdot) \in L^2$ for almost every x. Since $(H_0 - E)^{-1}$ has integral kernel G_0 with $G_0(x, \cdot) \in L^2$ for almost all x, $(H - E)^{-1}$ has an integral kernel with

$G(x, \cdot; E) \in L^2$ a.e. in x. The integral equation (c) is just a translation of $(H - E)^{-1} = (H_0 - E)^{-1} - (H_0 - E)^{-1}V(H - E)^{-1}$. In particular, if Re E is sufficiently negative, the integral equation can be solved by iteration. For such E, (b) follows from the analogous properties of G_0 and the fact that V is real. Thus (b) holds for all $E \notin \sigma(H)$ by analytic continuation. It remains to show that $G(x, \cdot; E) \in L^1$ a.e. in x. This can be done by using the integral equation (Problem 61b). ▌

G is called the **Green's function** for H.

(IV) *Positive eigenvalues* As another preliminary, we need the fact:

Lemma 2 If $E > 0$ and $E \notin \mathscr{E}$, then E is not an eigenvalue of H.

This is left to the reader (Problem 62 or see the reference in the Notes). It implies that whenever $[\alpha, \beta] \cap \mathscr{E} = \emptyset$, $P_{[\alpha, \beta]} = P_{(\alpha, \beta)}$ so that the term $\frac{1}{2}[P_{[\alpha, \beta]} + P_{(\alpha, \beta)}]$ in Stone's formula is $P_{(\alpha, \beta)} = P_{[\alpha, \beta]}$.

(V) *The relation of $\#$ and the resolvent* Suppose Im $\kappa > 0$ and Re $\kappa \neq 0$. Since $G(x, \cdot; \kappa^2) \in L^1$, it has an inverse Fourier transform $g(x, k; \kappa) \equiv (2\pi)^{-3/2} \int G(x, y; \kappa^2)e^{ik \cdot y}\, d^3y$ which is continuous. Define $h(x, k; \kappa) \equiv (2\pi)^{3/2}(|k|^2 - \kappa^2)g(x, k; \kappa)$. Then the integral equation for G translates into an integral equation for h (after a side argument which allows the interchange of the Fourier transform integral and the integral equation integral):

$$h(x, k; \kappa) = e^{ik \cdot x} - \frac{1}{4\pi} \int \frac{e^{i\kappa|x-y|}}{|x - y|} V^{1/2}(y)p(y, k; \kappa)\, dy \tag{85a}$$

$$p(y, k; \kappa) = |V(y)|^{1/2}e^{ik \cdot y} - \frac{1}{4\pi} \int |V(y)|^{1/2} \frac{e^{i\kappa|x-y|}}{|x - y|} V^{1/2}(x)p(x, k; \kappa)\, dx \tag{85b}$$

The key fact is the relation between (85b) and the modified Lippmann–Schwinger equation (84). If $k \in \mathbb{R}^3$ is fixed and $\kappa = |k|$, the equation for $p(\cdot, k; \kappa)$ becomes identical to the equation for $\psi(\cdot, k)$. This can be used to prove:

Lemma 3 Let $f \in C_0^\infty(\mathbb{R}^3)$. Then the integrals

$$\Phi(k; \kappa) = (2\pi)^{-3/2} \int \overline{h(x, k; \kappa)} f(x)\, d^3x$$

and

$$f^*(k) = (2\pi)^{-3/2} \int \overline{\varphi(x, k)} f(x)\, d^3x$$

converge absolutely if $\operatorname{Im} \kappa > 0$ in the Φ integral or if $|k|^2 \notin \mathscr{E}$ in the f^* integral. Suppose that $[\alpha, \beta] \cap \mathscr{E} = \varnothing$ with $\alpha > 0$. Then $\Phi(k; \kappa)$ has an extension to the region $\alpha^{1/2} \leq \operatorname{Re} \kappa \leq \beta^{1/2}$, $\operatorname{Im} \kappa \geq 0$, which is uniformly continuous in k and κ, and for $k^2 \in [\alpha, \beta]$

$$f^*(k) = \Phi(k;\ |k|)$$

We thus have related f^* to the boundary value of the resolvent.

(VI) *Proof of (82e′) when $f \in C_0^\infty$:*

Lemma 4 Let $f \in C_0^\infty$ and let $[\alpha, \beta] \cap \mathscr{E} = \varnothing$ with $\alpha > 0$. Then

$$\|P_{[\alpha, \beta]} f\|^2 = \int_{\alpha^{1/2} < |k| < \beta^{1/2}} |f^*(k)|^2\, d^3k$$

Proof Again, we shall not provide the technical details. Let $\kappa^2 = \mu + i\varepsilon$ with $\varepsilon > 0$, and $\operatorname{Im} \kappa > 0$. Up to a factor of $(2\pi)^{3/2}(|k|^2 - \mu - i\varepsilon)$, $h(x, \cdot; \kappa)$ is the Fourier transform of $G(x, \cdot; \kappa^2)$ so the Plancherel theorem implies that

$$\begin{aligned}(\kappa^2 - \bar{\kappa}^2) &\int \overline{G(z, x; \bar{\kappa}^2)} G(z, y, \bar{\kappa}^2)\, dz \\ &= \int \frac{2i\varepsilon}{(k^2 - \mu)^2 + \varepsilon^2} h(x, k; \kappa) \overline{h(y, k; \kappa)}\, \frac{dk}{(2\pi)^3} \end{aligned} \tag{86}$$

If we multiply the left-hand side of (86) by $\overline{f(x)} f(y)$ and integrate, we obtain

$$(\kappa^2 - \bar{\kappa}^2)(R_{\bar{\kappa}^2} f, R_{\bar{\kappa}^2} f) = (\kappa^2 - \bar{\kappa}^2)(f, R_{\kappa^2} R_{\bar{\kappa}^2} f) = (f, R_{\kappa^2} - R_{\bar{\kappa}^2} f)$$

where $R_E \equiv (H - E)^{-1}$. On the other hand, the right-hand side of (86) then becomes

$$\int \frac{2i\varepsilon}{(|k|^2 - \mu)^2 + \varepsilon^2} |\Phi(k; \sqrt{\mu + i\varepsilon})|^2\, dk$$

We thus conclude that

$$\int_\alpha^\beta (f, [R_{\mu+i\varepsilon} - R_{\mu-i\varepsilon}]f)\frac{d\mu}{2\pi i} = \frac{1}{\pi}\int_\alpha^\beta \int \frac{\varepsilon}{(|k|^2-\mu)^2+\varepsilon^2}\,|\Phi(k, \sqrt{\mu+i\varepsilon})|^2\,d\mu\,dk \tag{87}$$

As $\varepsilon \to 0$, Stone's formula and Lemma 2 imply that the left-hand side of (87) approaches $(f, P_{[\alpha,\beta]}f) = \|P_{[\alpha,\beta]}f\|^2$. Formally, $\varepsilon\pi^{-1}[(|k|^2-\mu)^2+\varepsilon^2]^{-1}$ approaches $\delta(k^2 - |\mu|)$ as $\varepsilon \to 0$ (see (V.4)), so that one can show that the right side of (87) approaches $\int_{\alpha<|k^2|<\beta} |f^*(k)|^2\,dk$ by using Lemma 3. ∎

(VII) *Extension to general f* Using Lemma 4, polarization, and a variety of limiting arguments, it is now easy to prove the remainder of Theorem XI.41 with the three exceptions: (i) Ran $\# = L^2$, (ii) $(\Omega^+ f)^* = \hat{f}$, and (iii) equation (82b). At this stage the formula (82b) is only proven in weak form. Once it is proven that Ran $\# = L^2$, we then get (82b). For details, see the reference in the Notes.

(VIII) *Reduction to (88)* Suppose that we can prove

$$\widehat{((\Omega^+)^* f)} = f^* \tag{88}$$

Then (83) follows from

$$(\Omega^+ f)^* = \widehat{(\Omega^+)^*\Omega^+ f} = \hat{f}$$

and Ran $\# = L^2$ follows from the fact that ^ and $(\Omega^+)^*$ are surjective. Thus proving (88) completes the proof of Theorem XI.41.

(IX) *Aside on abelian limits* To prove (88) we need the following:

Lemma 5 Let $f(x)$ be a bounded measurable function and suppose that $\lim_{t\to\infty} \int_0^t f(x)\,dx = a$. Then $\lim_{\varepsilon \downarrow 0} \int_0^\infty e^{-\varepsilon s} f(s)\,ds = a$.

Proof Let $g(t) = \int_0^t f(s)\,ds$ and $q(\varepsilon) = \int_0^\infty e^{-\varepsilon s} f(s)\,ds$. Then $g'(t) = f(t)$ a.e., so an integration by parts proves that

$$q(\varepsilon) = \int_0^\infty \varepsilon e^{-\varepsilon s} g(s)\,ds$$

Using the facts that g is bounded, $g(t) \to a$ as $t \to \infty$, and $\int_0^\infty \varepsilon e^{-\varepsilon s}\,ds = 1$, it is easy to prove that $q(\varepsilon) \to a$ (Problem 63). ∎

(X) *Conclusion* We are ready to conclude our sketch of the proof of Theorem XI.41.

Proof of (88) We need only prove the result for $f \in \mathscr{H}_{\text{ac}}$, the absolutely continuous space for H. For, if $f \in \mathscr{H}_{\text{ac}}^{\perp}$, then $(\Omega^+)^* f = 0$ and, by (82e) proven in VII, $f^\# = 0$. Thus it is sufficient to prove that

$$(f, \Omega^+ g) = \int \overline{f^\#(k)} \hat{g}(k)\, dk \tag{89}$$

for a set of g dense in $\mathscr{H}$ and a set of f dense in $\mathscr{H}_{\text{ac}}$. We shall suppose that $f^\#$ has support in some interval $[\alpha, \beta]$ disjoint from $\mathscr{E}$ and that $g \in C_0^\infty$. In the computations below we shall not use these technical assumptions on f and g explicitly, but we shall interchange limits and multiple integrals; in justifying these interchanges the technical assumptions on f and g are useful.

Since $f, g \in Q(H) = Q(H_0)$, by Problem 20,

$$(f, \Omega^+ g) - (f, g) = i \lim_{t \to -\infty} \int_0^t (f, e^{iHs} V e^{-iH_0 s} g)\, ds$$

Thus, by Lemma 5,

$$(f, \Omega^+ g) = (f, g) + i \lim_{\varepsilon \downarrow 0} \int_0^{-\infty} (f, e^{iHt} V e^{-iH_0 t} g) e^{\varepsilon t}\, dt \tag{90}$$

From (82e′), it is easy to prove that $(f, e^{iHt} g) = \int \overline{f^\#(k)} e^{ik^2 t} g^\#(k)\, dk$ if either f or g is in $\mathscr{H}_{\text{ac}}$. As a result

$$\begin{aligned}(f, e^{iHt} V e^{-iH_0 t} g) &= \int \overline{f^\#(k)} e^{ik^2 t} (V e^{-iH_0 t} g)^\#(k)\, dk \\ &= (2\pi)^{-3/2} \iint \overline{f^\#(k)} e^{ik^2 t} \overline{\varphi(x, k)} V(x) (e^{-iH_0 t} g)(x)\, dx\, dk\end{aligned}$$

Thus

$$\begin{aligned}&\int_0^{-\infty} (f, e^{iHt} V e^{-iH_0 t} g) e^{\varepsilon t}\, dt \\ &\quad = (2\pi)^{-3/2} \int_0^{-\infty} \iint \overline{f^\#(k) \varphi(x, k)} V(k) (e^{-it(H_0 - k^2 + i\varepsilon)} g)(x)\, dx\, dk\, dt \\ &\quad = -i(2\pi)^{-3/2} \iint \overline{f^\#(k) \varphi(x, k)} V(x) [(H_0 - k^2 + i\varepsilon)^{-1} g](x)\, dx\, dk \\ &\quad = \frac{-i}{4\pi} (2\pi)^{-3/2} \iiint \overline{f^\#(k) \varphi(x, k)} V(x) \frac{e^{-i|x-y|\sqrt{k^2 - i\varepsilon}}}{|x - y|} g(y)\, dx\, dy\, dk\end{aligned}$$

Taking $\lim_{\varepsilon \downarrow 0}$ inside the integral in (90), we see that

$$\begin{aligned}(f, \Omega^+ g) &= (f, g) + (2\pi)^{-3/2} \iint \overline{f^*(k)} g(y) \\ &\qquad \times \left[\frac{1}{4\pi} \int \frac{e^{-ik|x-y|}}{|x-y|} V(x) \overline{\varphi(x, k)}\, dx\right] dk\, dy \\ &= (f, g) + (2\pi)^{-3/2} \int \overline{f^*(k)} g(y) [e^{-ik \cdot y} - \overline{\varphi(y, k)}]\, dk\, dy \\ &= (f, g) + \int \overline{f^*(k)} \hat{g}(k)\, dk - \int \overline{f^*(k)} g^*(k)\, dk \\ &= \int \overline{f^*(k)} \hat{g}(k)\, dk\end{aligned}$$

In the second line above we used the Lippmann–Schwinger equation and at the last step we used (82e). This completes the proof of (89) and so of (88). Our sketch of the proof of Theorem XI.41 is thus concluded. ▮

The Lippmann–Schwinger eigenfunctions $\varphi(x, k)$ are especially useful because they can be used to express the S-matrix. First, we introduce an auxiliary object:

Definition Let $\mathbf{k} \in \mathbb{R}^3$, $\mathbf{k}' \in \mathbb{R}^3$, $k'^2 \notin \mathscr{E}$. Define

$$T(\mathbf{k}, \mathbf{k}') = (2\pi)^{-3} \int e^{-i\mathbf{k} \cdot \mathbf{x}} V(\mathbf{x}) \varphi(\mathbf{x}, \mathbf{k}')\, d\mathbf{x}$$

$T(\cdot, \cdot)$ is called the ***T*-matrix.**

Theorem XI.42 $T(\mathbf{k}, \mathbf{k}')$ is uniformly continuous in any region of the form $\mathbb{R}^3 \times \{\mathbf{k}' \mid k'^2 \in [\alpha, \beta]\}$ where $\alpha > 0$ and $[\alpha, \beta] \cap \mathscr{E} = \varnothing$. Moreover, if $f, g \in \mathscr{S}(\mathbb{R}^3)$ where $\hat{f}$ and $\hat{g}$ are functions with supports in spherical shells disjoint from $\{\mathbf{k}' \mid k'^2 \in \mathscr{E}\}$, then

$$(f, (S - I)g) = (-2\pi i) \int \overline{\hat{f}(\mathbf{k})} \hat{g}(\mathbf{k}') T(\mathbf{k}, \mathbf{k}')\, \delta(k^2 - (k')^2)\, d\mathbf{k}\, d\mathbf{k}' \qquad (91)$$

Before proving Theorem XI.42, we make a series of remarks. First, the $\delta(k^2 - (k')^2)$ in (91) is a shorthand way of writing

$$\int \overline{\hat{f}(\mathbf{k})} \left[\int_{k'^2 = k^2} T(\mathbf{k}, \mathbf{k}') \hat{g}(\mathbf{k}') (\tfrac{1}{2} k')\, d\Omega(\mathbf{k}')\right] d\mathbf{k}$$

where $d\Omega(\mathbf{k}')$ is the angular measure on the sphere and $\frac{1}{2}k'$ is the Jacobian of the coordinate change from $\mathbf{k}'$ to $\langle (k')^2, \Omega(\mathbf{k}')\rangle$. (91) is often written symbolically as

$$S(\mathbf{k}, \mathbf{k}') = \delta(k - k') - 2\pi i T(\mathbf{k}, \mathbf{k}')\, \delta(k^2 - (k')^2)$$

This is a realization of the scheme discussed at the end of Section 5.

We also note that the set of f and g allowed in (91) is dense in L^2, so that φ completely determines S. Notice that S is completely determined by the values of $T(\mathbf{k}, \mathbf{k}')$ when $k = k'$. This set of values is known as the "on-shell T-matrix" or as the T-matrix "on the energy shell." It is a typical occurrence in physical theories, and in particular occurs in perturbation theoretic quantum field theory, that scattering is described in terms of an "on-shell" quantity which the theory also determines "off-shell." One of the beauties of Faddeev's three-body theory is that the *off-shell* T-matrix for the two-body system enters the theory of three-body scattering. We shall not have a chance to discuss this further.

Proof of Theorem XI.42 Since $S = (\Omega^-)^*\Omega^+$ and $I = (\Omega^+)^*\Omega^+$,

$$\begin{aligned}
(f, (S - I)g) &= (f, (\Omega^- - \Omega^+)^*\Omega^+ g) \\
&= ((\Omega^- - \Omega^+)f, \Omega^+ g) \\
&= \lim_{T\to\infty} \int_{-T}^{T} (e^{iHt}(iV)e^{-iH_0t}f, \Omega^+ g)\, dt \\
&= \lim_{\varepsilon\downarrow 0}(-i) \int_{-\infty}^{\infty} e^{-\varepsilon|t|}(e^{iHt}Ve^{-iH_0t}f, \Omega^+ g)\, dt \\
&= \lim_{\varepsilon\downarrow 0}(-i) \int_{-\infty}^{\infty} e^{-\varepsilon|t|} \\
&\quad \times \left(\int \overline{[e^{iHt}Ve^{-iH_0t}f]^*(k')}[\Omega^+ g]^*(k')\, dk' \right) dt
\end{aligned} \tag{92}$$

In the next to the last step we used Lemma 5, and in the last step we have used (82e) of Theorem XI.41 and the fact that $\Omega^+ g \in \mathscr{H}_{\mathrm{ac}}$. By (83),

$$(\Omega^+ g)^*(k') = \hat{g}(k')$$

and by (82),

$$\begin{aligned}
[e^{iHt}Ve^{-iH_0t}f]^*(k') &= e^{i|k'|^2t}[Ve^{-iH_0t}f]^*(k') \\
&= (2\pi)^{-3/2} \int e^{i|k'|^2t}V(x)(e^{-iH_0t}f)(x)\overline{\varphi(x, k')}\, dx \\
&= (2\pi)^{-3} \int e^{i[|k'|^2 - |k|^2]t}V(x)e^{ik\cdot x}\overline{\varphi(x, k')}\hat{f}(k)\, dx\, dk
\end{aligned}$$

Thus the expression in (92) is

$$(-i)(2\pi)^{-3}\int_{-\infty}^{\infty} dt\left[\iint e^{i(|k|^2-|k'|^2)t-\varepsilon|t|}V(x)\varphi(x,k')e^{-ik\cdot x}\overline{\hat{f}(k)}\hat{g}(k')\,dk'\,dx\,dk\right]$$

Doing the t-integration,

$$(f,(S-I)g)=\lim_{\varepsilon\downarrow 0}\int(-i)T(k,k')\frac{2\varepsilon}{(|k|^2-|k'|^2)^2+\varepsilon^2}\overline{\hat{f}(k)}\hat{g}(k')\,dk\,dk' \tag{93}$$

By definition, $T(k, k')$ is the inner product of $f_k(x) = (2\pi)^{-3}e^{-ik\cdot x}V^{1/2}(x)$ and $\psi(x, k')$. Since $\psi(\cdot, k')$ is uniformly L^2-continuous in the regions considered and $f_k(\cdot)$ is uniformly L^2-continuous since $V \in L^1$, $T(k, k')$ has the claimed continuity properties. As a result, the formula, $2\varepsilon[((|k|^2 - |k'|^2) + \varepsilon^2]^{-1} \to 2\pi\,\delta(|k|^2 - |k'|^2)$ valid as measures on $\kappa(\mathbb{R}^6)$ can be applied to (93). This completes the proof of (91). ▮

There is an alternative proof to this theorem in certain circumstances; see the third appendix to Section 8 or Problem 67.

Now that we have the connection between the eigenfunctions and S, we can develop the theory in various directions. Since φ obeys the Lippmann–Schwinger equation (81), there is a formal series for φ by iteration and thus a series for T:

$$T(\mathbf{k},\mathbf{k}')=\sum_{n=0}^{\infty}T_n(\mathbf{k},\mathbf{k}') \tag{94a}$$

$$T_0(\mathbf{k},\mathbf{k}')=(2\pi)^{-3}\int e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}}V(x)\,dx \tag{94b}$$

$$\begin{aligned}T_n(k,k')=(2\pi)^{-3}(-1)^n(4\pi)^{-n}\int e^{-i\mathbf{k}\cdot\mathbf{x}_0}V(\mathbf{x}_0)\\ \times\frac{e^{ik'|\mathbf{x}_0-\mathbf{x}_1|}}{|\mathbf{x}_0-\mathbf{x}_1|}V(\mathbf{x}_1)\frac{e^{ik'|\mathbf{x}_1-\mathbf{x}_2|}}{|\mathbf{x}_1-\mathbf{x}_2|}V(\mathbf{x}_2)\\ \cdots V(\mathbf{x}_{n-1})\frac{e^{ik'|\mathbf{x}_{n-1}-\mathbf{x}_n|}}{|\mathbf{x}_{n-1}-\mathbf{x}_n|}V(\mathbf{x}_n)e^{i\mathbf{k}'\cdot\mathbf{x}_n}\,dx_0\cdots dx_n\end{aligned}$$

The series (94b) is called the **Born series** for T and the leading term (94b) is called the **Born amplitude**. Because of our study of $\mathscr{E}$ ((II) in the sketch of the proof of Theorem XI.41; see also Problem 60), we can easily prove that in certain cases the Born series converges

Theorem XI.43 Let $V \in L^1 \cap R$.

(a) There exists a number K so that the Born series for $T(\mathbf{k}, \mathbf{k}')$ converges if $(k')^2 > K^2$, $\mathbf{k} \in \mathbb{R}^3$.
(b) If $\|V\|_R^2 < 4\pi$, then the Born series for $T(\mathbf{k}, \mathbf{k}')$ converges for all $\mathbf{k}$, $\mathbf{k}' \in \mathbb{R}^3$.

Proof $T(k, k')$ is the inner product of a fixed L^2-vector with the modified Lippmann–Schwinger function $\psi(x, k') = |V(x)|^{1/2}\varphi(x, k')$. ψ obeys an L^2 integral equation whose iteration leads to the Born series. If the series for ψ converges in L^2 for some k', then the Born series converges for that value of k' and all k. To show that the series for ψ converges, it is enough to show that the kernel of the integral equation it satisfies is the kernel of an integral operator $K_{k'}$ with norm less than 1. For $V \in R$, we know that $\lim_{k' \to \infty} \|K_{k'}\| = 0$ (Problem 60), so (a) holds. If $\|V\|_R^2 < 4\pi$, then $\|K_{k'}\|_{\text{H.S.}} = (4\pi)^{-1/2}\|V\|_R < 1$ for all k'. ∎

Using the methods of Section 7, it can be shown that if $V \in R$ and if $S(\lambda)$ is the S-operator for $-\Delta + \lambda V$, λ real, then $S(\lambda)$ has an operator-valued analytic continuation to the region $\{\lambda \mid |\lambda| \, \|V\|_R < 4\pi\}$. Theorem XI.43 is just one of many results about recovering S from a Born series or from some other formal series. Using the Fredholm theory for solving L^2 equations with Hilbert–Schmidt kernels, one can find convergent series $N(\mathbf{k}, \mathbf{k}')$ and $D(k')$ with $D(\alpha) \neq 0$ if $\alpha^2 \notin \mathscr{E}$ so that $T(\mathbf{k}, \mathbf{k}') = N(\mathbf{k}, \mathbf{k}')/D(k')$. This realization of T is the start of an analysis of the convergence of the Padé approximants formed from the Born series. This summability method can be shown to converge in some cases where the Born series diverges (see the Notes). In addition, there are a variety of results concerning convergence of series for the "partial wave amplitudes" discussed in Section 8.

A second consequence of the relation between T and S is the *unitarity relation for* T, (95).

Theorem XI.44 Let $V \in L^1 \cap R$ and suppose that $\alpha^2 \notin \mathscr{E}$. Then for any $\mathbf{k}, \mathbf{k}' \in R^3$ with $k = k' = \alpha$,

$$\operatorname{Im} T(k, k') = \pi \int \overline{T(k'', k)}T(k'', k')\, \delta((k'')^2 - \alpha)\, d^3k'' \tag{95}$$

Proof Since $\mathscr{E}$ is closed, we can find β, γ with $\alpha \in (\beta, \gamma)$ and $[\beta^2, \gamma^2] \cap \mathscr{E} = \varnothing$. By Theorem XI.42, if f is in $\mathscr{S}$ and $\hat{f}$ has support in $F = \{\mathbf{k} \mid \beta < k < \gamma\}$, then $\widehat{(Sf)}(k) = \hat{f}(k) - (2\pi i)\int T(k, k')\hat{f}(k')\,\delta(k^2 - k'^2)\, dk'$. By a simple limiting argument, this formula holds if $\hat{f}$ is merely continuous (with support in F) and the map $M: \hat{f} \mapsto \widehat{Sf}$ takes the continuous functions with support in F into themselves. The adjoint of M is clearly given by

$$(M^*g)(k) = g(k) + (2\pi i) \int \overline{T(k', k)} g(k')\, \delta(k^2 - k'^2)\, dk'$$

The relation $M^*M = 1$, which follows from $S^*S = I$, implies that for almost all pairs $\langle k, k' \rangle$ with $|k| = |k'|$ and $k, k' \in F$, (95) holds. Since both sides are continuous in $\langle k, k' \rangle$ in the region $\{\langle k, k' \rangle \in F \times F \mid |k| = |k'|\}$, (95) holds throughout the region. ▌

To understand the importance of the unitarity relation for T, we must understand what quantity is measured in a scattering experiment. For simplicity, we suppose that V is spherically symmetric so that $T(\mathbf{k}, \mathbf{k}')$ depends only on k, k' and $\mathbf{k} \cdot \mathbf{k}'$. Given k and $\cos\theta \in [-1, 1]$, find $\mathbf{k}, \mathbf{k}'$ with $k' = k$ and $\mathbf{k} \cdot \mathbf{k}' = k^2 \cos\theta$. Then, the **scattering amplitude** $f(k, \theta)$ is defined by

$$f(k, \theta) \equiv -2\pi^2 T(\mathbf{k}, \mathbf{k}') \tag{96}$$

An argument which is partially heuristic and which we summarize in the Notes shows that if one sends in a beam of particles of energy $E = k^2$, the differential cross section (see Section 2) is given by

$$d\sigma/d\Omega = |f(k, \theta)|^2 \tag{97a}$$

The total cross section is thus given by

$$\sigma \equiv \int \frac{d\sigma}{d\Omega}\, d\Omega = 2\pi \int_{-\pi}^{\pi} |f(k, \theta)|^2 \sin\theta\, d\theta \tag{97b}$$

If we write the unitarity relation with $\mathbf{k} = \mathbf{k}'$, then it says

$$\operatorname{Im} T(\mathbf{k}, \mathbf{k}) = \frac{\pi|\mathbf{k}|}{2} \int |T(\mathbf{k}'', \mathbf{k})|^2\, d\Omega(\mathbf{k}'')$$

or that

$$\sigma = \frac{4\pi}{k} \operatorname{Im} f(k, 0) \tag{97c}$$

The relation (97c) is often called the **optical theorem**. Physically, it is an expression of the fact that the amount scattered out of the beam (the left-hand side of (97c)) must be compensated for by the interference between the original beam and the forward scattered wave (the right-hand side of (97c)).

We thus see that only the magnitude of f is directly measurable via (97a). Unitarity provides a partial handle for determining the argument of f. For example, using (97c) one can determine $\arg f(k, 0)$ up to an ambiguity of reflection about the imaginary axis if one knows $(d\sigma/d\Omega)(k, \theta)$ for all θ. And, in fact, we saw in Section V.6 that if $d\sigma/d\Omega$ is sufficiently "small," then unitarity and the differential cross section determine f uniquely, for all θ.

Appendix to XI.6: Introduction to eigenfunction expansions by the auxiliary space method

In this section we developed eigenfunction expansions by solving a modified Lippmann–Schwinger equation in L^2. It is often useful to follow a somewhat different path which depends on a Banach space X which is continuously imbedded as a dense subspace $X \subset \mathscr{H}$. Under this situation we can naturally imbed $\mathscr{H}$ into X^* and thus X into X^* using the duality of $\mathscr{H}$; that is, for $\varphi \in \mathscr{H}$, define $\ell_\varphi \in X^*$ by $\ell_\varphi(x) = (\varphi, x)$. The triple $X \subset \mathscr{H} \subset X^*$ is reminiscent of the construction of $\mathscr{H}_1 \subset \mathscr{H} \subset \mathscr{H}_{-1}$ in the theory of quadratic forms (Theorem VIII.15).

Given the triple $X \subset \mathscr{H} \subset X^*$ one tries to obtain an eigenfunction expansion by a two-step process: (i) Show that $(H - z)^{-1}\colon X \to X^*$ extends continuously from $\operatorname{Im} z > 0$ to the real axis or the real axis with an exceptional set removed. (ii) Use the operators $(H - k^2 - i0)^{-1}$ to obtain generalized eigenfunctions $\varphi \in X^*$. (i) implies that $(f, (H - z)^{-1}f)$ has an extension to the real axis for $f \in X$; and, as we shall see in Section XIII.6, this implies that H has no singular continuous spectrum. For this reason, just developing step (i) is of considerable interest; we shall make just this kind of development in Section XIII.8 for a very large class of operators $-\Delta + V$ using rather subtle arguments. Here we want to illustrate the ideas of (i) by taking the extremely special situation where V falls off exponentially. We shall then describe step (ii) for the case where we are, in addition, in one dimension. The Notes give extensive references to the theory in more general circumstances.

Let X_a be the Hilbert space of functions with $e^{a|x|}f \in L^2 \equiv \mathscr{H}$ with the natural norm. Then for $a > 0$, $X_a \subset \mathscr{H} \subset X_{-a} = X_a^*$ as above. We first claim:

Lemma 1 The function $(-\Delta - k^2)^{-1}\colon X_a \to X_{-a}$, defined for $\operatorname{Im} k > 0$, extends analytically to the region $\operatorname{Im} k > -a$, $\arg k \neq -\frac{1}{2}\pi$, as an analytic function with values in the compact operators from X_a to X_{-a}. The same thing is true of the functions $\partial_i(-\Delta - k^2)^{-1}$.

Proof Let $G_0(x, y; E)$ be the integral kernel of $(-\Delta - E)^{-1}$ for $E \notin [0, \infty)$ defined uniquely for all x, y with $x \neq y$ by demanding continuity. We first claim that $G_0(x, y; E)$ extends analytically to all $\sqrt{E}$ with $\arg(\sqrt{E}) \neq -\frac{1}{2}\pi$ and obeys the estimate

$$|G_0(x, y; E)| \le C_{\varepsilon,\delta}(|x-y|^{-(n-2)} + E^{(n-2)/2})e^{|x-y|(|\operatorname{Im}\sqrt{E}|+\varepsilon|E|^{1/2})} \tag{98}$$

if $n \ge 3$ and $(\operatorname{Re}\sqrt{E})/|\sqrt{E}| \ge \delta$. If $n = 1$, a similar estimate holds with no $|x-y|^{-(n-2)}$ term; and if $n = 2$, the term before the exponential is replaced by $|\ln(|x-y|^{-1}E^{1/2})| + 1$. (98) is obvious if $n = 3$ or $n = 1$ from the explicit form that G_0 takes. For general n, the proof of (98), which is *not* the best possible estimate, is left to the reader (Problem 65).

Let $H(x, y; k)$ be the function $e^{-a|x|}G_0(x, y; k^2)e^{-a|y|}$. By (98), for any k with $\operatorname{Im} k > -a$, $\arg k \neq -\frac{1}{2}\pi$,

$$|H(x, y; k)| \le h_k(x-y)$$

with $h_k \in L^1$. For $n \ge 3$, $h_k(x) = \text{const } |x-y|^{-(n-2)}e^{-\gamma|x|}$; for $n = 2$, $h_k(x) = \text{const } (|\ln|x|| + 1)e^{-\gamma|x|}$; and, for $n = 1$, $h_k(x) = \text{const } e^{-\gamma|x|}$. It follows by Young's inequality that $H(x, y; k)$ is the kernel of a bounded integral operator. The operator is clearly analytic in k and, by Theorem IX.20, it is compact for $\operatorname{Im} k > 0$ and so for all k by analytic continuation and the fact that the compact operators are norm closed. Thus, $e^{-a|x|}(-\Delta - k^2)^{-1}e^{-a|y|}$ is an analytic function with values in the compact operators on L^2 for $\operatorname{Im} k > -a$, $\arg k \neq -\pi$. Since $e^{\pm a|x|}$ is a unitary map from L^2 to $X_{\mp a}$, the result is proven. The $\partial_i(-\Delta - k^2)^{-1}$ result is left to the reader (Problem 65). ▌

Now suppose that $|V(x)| \le ce^{-2a|x|}$. Then clearly $V\colon X_{-a} \to X_a$ is bounded so that $V(-\Delta - k^2)^{-1}$ is, for each k, a compact operator from X_a to itself. Moreover, $\eta = -V(-\Delta - k^2)^{-1}\eta$ has no solutions in X_a for $\operatorname{Im} k > 0$, $\arg k \neq \frac{1}{2}\pi$ since it has no solutions in L^2 for, if $\varphi \in L^2$ obeys the equation, then $\psi = (-\Delta - k^2)^{-1}\varphi$ is in $D(H)$ and obeys $(-\Delta + V)\psi = k^2\psi$. It follows by the analytic Fredholm theorem that except for a discrete set $\mathscr{E} \subset \mathbb{R}$, $(1 + V(-\Delta - k^2)^{-1})^{-1}$ has an analytic continuation from $\operatorname{Im} k > 0$ to a neighborhood N of $\mathbb{R}$ with $\mathscr{E}$ removed. Since $(H - k^2)^{-1} = (-\Delta - k^2)^{-1}(1 + V(-\Delta - k^2)^{-1})^{-1}$, we have proven case (a) of the following theorem. We shall use case (b) in Section 11.

Theorem XI.45 Let H be one of the following operators on $L^2(\mathbb{R}^n)$:

(a) $H = -\Delta + V$ with $|V(x)| \le Ce^{-2a|x|}$.

(b) $H\eta = -\alpha\nabla \cdot \beta\nabla(\alpha\eta)$ with α and β strictly positive functions so that $\alpha - \alpha_0$, $\beta - \beta_0 \in C_0^\infty$ for suitable constants α_0, $\beta_0 > 0$.

Then H is self-adjoint on $D(-\Delta)$ and there is a discrete set $\mathscr{E} \subset \mathbb{R}$ and a neighborhood N of $\mathbb{R}$ so that $(H - k^2)^{-1}$ has a continuation as an analytic $\mathscr{L}(X_a, X_{-a})$-valued function from the region $\{k \,|\, \operatorname{Im} k > 0,\ -k^2 \text{ not an eigenvalue of } H\}$ to $N \backslash \mathscr{E}$. a is arbitrary in case (b).

Proof We need only prove case (b). By using Leibnitz' rule, we can write

$$H = -f\Delta + \mathbf{g} \cdot \nabla + h$$

where $\mathbf{g}$, h, $f_1 \equiv f - f_0 \in C_0^\infty$ and $f_0 = \alpha_0^2 \beta_0$. Moreover, $f = \alpha^2 \beta$ is strictly positive. That H is self-adjoint on $D(-\Delta)$ is a simple application of Theorem X.13 which we leave to the reader (Problem 66). Let $V = H - H_0$; $H_0 = -f_0 \Delta$. As above, the theorem will be proven if we show that $(1 + V(H_0 - k^2)^{-1})^{-1}$ is an analytic $\mathscr{L}(X_a, X_a)$-valued function. $V(H_0 - k^2)^{-1}$ is not compact but, if $W = g \cdot \nabla + h$, then

$$\begin{aligned} 1 + V(H_0 - k^2)^{-1} &= (H_0 + V - k^2)(H_0 - k^2)^{-1} \\ &= [ff_0^{-1}(H_0 - k^2) + W + k^2 f_1 f_0^{-1}](H_0 - k^2)^{-1} \\ &= ff_0^{-1} + [(W + k^2 f_1 f_0^{-1})(H_0 - k^2)^{-1}] \\ &= (ff_0^{-1})[1 + (f^{-1} f_0 W + f^{-1} f_1 k^2)(H - k^2)^{-1}] \end{aligned}$$

The expression in $[\cdots]$ is I plus an analytic function with values in the compact operators in $\mathscr{L}(X_a)$, so $I + V(H_0 - k^2)^{-1}$ is invertible except on a discrete set by Theorem VI.14. ▮

We now turn to producing eigenfunction expansions for $-d^2/dx^2 + V(x)$ with $|V(x)| \le Ce^{-2a|x|}$. The key to all such expansions is the following heuristic formula:

$$\operatorname{Im}(H - k^2 - i0)^{-1} = W(k)^* [\operatorname{Im}(H_0 - k^2 - i0)^{-1}] W(k) \tag{99}$$

where

$$W(k) = (1 + V(H_0 - k^2 - i0)^{-1})^{-1}$$

and

$$\operatorname{Im}(A - k^2 - i0)^{-1} = \lim_{\varepsilon \downarrow 0} (2i)^{-1}[(A - k^2 - i\varepsilon)^{-1} - (A - k^2 + i\varepsilon)^{-1}]$$

(99) is formally true because if $\operatorname{Im} z > 0$, if A is self-adjoint, and if $B = A + C$ is self-adjoint on $D(A)$, then

$$\begin{aligned}(B - z)^{-1} - (B - \bar{z})^{-1} &= 2(\operatorname{Im} z)(B - \bar{z})^{-1}(B - z)^{-1} \\ &= 2(\operatorname{Im} z)[(1 + C(A - z)^{-1})^{-1}]^*(A - \bar{z})^{-1} \\ &\quad \times (A - z)^{-1}(1 + C(A - z)^{-1})^{-1} \\ &= [(1 + C(A - z)^{-1})^{-1}]^* \\ &\quad \times [(A - z)^{-1} - (A - \bar{z})^{-1}](1 + C(A - z)^{-1})^{-1}\end{aligned} \tag{100}$$

so that (99) results if one can take $\operatorname{Im} z$ to zero. In the case at hand, (99) is valid for $k^2 \notin \mathscr{E}$ if we interpret $(H - k^2 - i0)^{-1}$ and $(H_0 - k^2 - i0)^{-1}$ as maps from X_a to X_{-a}, $W(k)$ as a map from X_a to X_a, and $W(k)^*$ as a map from X_{-a} to X_{-a}. For these interpretations can be made if $k^2 - i0$ is replaced by z with $\operatorname{Im} z > 0$, and all maps are analytic up to $k^2 + i0$ (except in $\mathscr{E}$) so that (100) implies (99).

To supplement (99) we need the fact that $H_0 = -d^2/dx^2$ has an eigenfunction expansion with eigenfunctions $\varphi_0(x, k) = e^{ikx}$. Notice that these eigenfunctions lie in X_{-a} and that since the kernel of $(H_0 - k^2 - i0)^{-1}$ is $\frac{1}{2}e^{ik|x-y|}$, we have that for $f \in X_a$,

$$\begin{aligned}&\operatorname{Im} (f, (H_0 - k^2 - i0)^{-1}f) \\ &\quad = \frac{1}{2} \iint \overline{f(x)} \sin(k(x - y))f(y)\, dx\, dy \\ &\quad = \tfrac{1}{2}[(f, \varphi_0(k))(\varphi_0(k), f) + (f, \varphi_0(-k))(\varphi_0(-k), f))]\end{aligned}$$

Defining $\varphi(k) = W(|k|)\varphi_0(k)$, we see by (99) that

$$\operatorname{Im}(f, (H - k^2 - i0)^{-1}f) = \frac{1}{2} \sum_{\delta = \pm 1} |(\varphi(\delta k), f)|^2$$

Using Stone's formula, we obtain that for $f \in X_a$ and $[a, b] \subset [0, \infty)\backslash\mathscr{E}$,

$$(f, P_{[a, b]}f) = \int_{a < k^2 < b} |f^*(k)|^2\, dk$$

where $f^*(k) = (2\pi)^{-1/2}(\varphi(k), f)$. From this point onward, the easy passage to the Plancherel relation and inversion formula for # and the connection with scattering theory are essentially identical to our discussion in Section 6.

XI.7 Quantum scattering IV: Dispersion relations

Rigorous proofs of dispersion relations are like breasts on a man, neither useful nor ornamental.
M. L. Goldberger

In agreement with the scheme presented at the conclusion of Section 5, we have seen that the two-body scattering operator has a "kernel," $\delta(\mathbf{k}-\mathbf{k}') - 2\pi i\delta(k^2-(k')^2)T(\mathbf{k},\mathbf{k}')$ where $T(\mathbf{k},\mathbf{k}')$ is continuous on $F \equiv \{\langle \mathbf{k},\mathbf{k}'\rangle \mid k^2 = (k')^2;\ k^2 \notin \mathscr{E}\}$. In this section we shall study T further. Our main goal will be to show that T is analytic in a suitable neighborhood of F when V lies in a somewhat restrictive class of potentials. To illustrate our method and to show that the analyticity of $T(\mathbf{k},\mathbf{k})$ is a general phenomenon, we first prove:

Theorem XI.46 Let V be in $L^1 \cap R$ and let $\mathbf{e}$ be a fixed unit vector in $\mathbb{R}^3$. Then, there exists a function $\tau_F(k)$ meromorphic in $\{k \mid \operatorname{Im} k > 0\}$ so that:

(a) If k_0 is real and $k_0^2 \notin \mathscr{E}$, then

$$\lim_{k\to k_0;\ \operatorname{Im} k>0} \tau_F(k) = T(k_0\mathbf{e}, k_0\mathbf{e})$$

The limit is uniform on compact subsets of $\mathbb{R}\backslash\mathscr{E}^{1/2}$.

(b) The only poles of τ_F in the upper half-plane occur on the imaginary axis at the points k where k^2 is an eigenvalue of $-\Delta + V$. Moreover all these poles are simple.

(c) $\tau_F(-\bar{k}) = \overline{\tau_F(k)}$.

(d) $\lim_{k\to\infty} \tau_F(k) = \tau_{\text{Born}} \equiv (2\pi)^{-3}\int V(x)\,dx$. The limit holds uniformly in the closed half-plane when τ_F is extended to $\mathbb{R}\backslash\mathscr{E}^{1/2}$

Proof For k real, define $\tau_F(k) = T(k\mathbf{e}, k\mathbf{e})$. We want to find some kind of continuation of $\tau_F(k)$ to the upper half-plane. We know that for k real

$$\tau_F(k) = (2\pi)^{-3}\int e^{-ik\mathbf{e}\cdot x} V^{1/2}(x)\psi(x, k\mathbf{e})\,dx \tag{101}$$

where ψ solves the modified Lippmann–Schwinger equation (84). The kernel of (84) can be continued to the upper half k plane, but the homogeneous term $|V(x)|^{1/2}e^{ik\mathbf{e}\cdot x}$ may not be in L^2 if $\operatorname{Im} k \neq 0$. Therefore, we further modify the Lippmann–Schwinger equation. Noticing that $e^{-ik\mathbf{e}\cdot x}\psi(x, k\mathbf{e})$ is the quantity that enters in (101), we define

$$\chi(x, k) = e^{-ik\mathbf{e}\cdot x}\psi(x, k\mathbf{e})$$

Then

$$\tau_F(k) = (2\pi)^{-3} \int V^{1/2}(x)\chi(x, k)\, dx \tag{102a}$$

and χ solves

$$\chi(x, k) = |V(x)|^{1/2} + \int M(x, y; k)\chi(y, k)\, dy \tag{102b}$$

with

$$\begin{aligned} &M(x, y; k) \\ &\quad = -(4\pi|x-y|)^{-1}|V(x)|^{1/2}V^{1/2}(y)\exp\{ik[|x-y| - e\cdot(x-y)]\} \end{aligned} \tag{102c}$$

Since $|(x-y)\cdot e| \le |x-y|$ for all x and y, $M(x, y; k)$ defines a Hilbert–Schmidt operator M_k for any k with $\operatorname{Im} k \ge 0$. A side argument (Problem 68) proves that $M_k\psi = \psi$ has a solution if and only if $K_k\varphi = \varphi$ has a solution where K_k is $-|V|^{1/2}(H_0 - k^2)^{-1}V^{1/2}$. It can also be shown that if $K_k\varphi = \varphi$ with $\operatorname{Im} k > 0$, then $\eta = (H_0 - k^2)^{-1}V^{1/2}\varphi \in Q(-\Delta + V)$ and $(H_0 + V)\eta = k^2\eta$ (Problem 69). Thus, by the analytic Fredholm theorem (Theorem VI.14), $(I - M_k)^{-1}$ exists except at the points k^2 that are eigenvalues of $-\Delta + V$ and $(I - M_k)^{-1}$ is meromorphic in the upper half-plane. Using the simplicity of the poles of $(-\Delta + V - k^2)^{-1}$, it can be shown that $(I - M_k)^{-1}$ has simple poles (Problem 71). For k in the upper half-plane, define

$$\tau_F(k) = (2\pi)^{-3}(V^{1/2}, (1 - M_k)^{-1}|V|^{1/2})$$

(a) and (b) are now easy.

As $k \to \infty$ in the closed half-plane, $\|M_k\| \to 0$ (see Problem 60), so (d) holds. Finally, if k is purely imaginary, each term in the series obtained by iterating (102b) is real-valued and the series converges if $|k|$ is large. Thus $\overline{\tau_F(-\bar{k})} = \tau_F(k)$ if $|k|$ is large and $\operatorname{Re} k = 0$. (c) follows by analytic continuation. ∎

In the case where V is spherically symmetric, τ_F is independent of **e** and $f(\mathbf{k}) = -2\pi^2\tau_F(\mathbf{k})$ is called the **forward scattering amplitude**. We saw in the last section that $\operatorname{Im}\tau_F(\mathbf{k})$ is determined by the total scattering cross section and unitarity. Interestingly enough, $\operatorname{Re}\tau_F(k)$ is determined by $\operatorname{Im}\tau_F(k)$ and a finite number of parameters, one for each bound state energy. For simplicity, consider the case where $\mathscr{E} = \varnothing$. Then:

Corollary If $V \in R \cap L^1(\mathbb{R}^3)$, if $\mathscr{E} = \varnothing$, and if we write $f(E) = -(2\pi)^2 \tau_F(\sqrt{E})$ for E real and positive, then

$$\operatorname{Re} f(E) = \mathscr{P} \int_0^\infty \frac{\operatorname{Im} f(E')}{E' - E} \frac{dE'}{\pi} + f_{\text{Born}} + \sum_{j=1}^n \frac{r_j}{E_j - E} \tag{103}$$

where $\mathscr{P} \int_0^\infty$ is the Cauchy principle value integral, $f_{\text{Born}} = -(4\pi)^{-1} \int V(x)\, dx$ and $E_1, \ldots, E_n$ are the bound states of $-\Delta + V$.

Sketch of proof This is a simple application of the analyticity of Theorem XI.46; the details are left to the reader (Problem 72). $f(E)$ is analytic in the plane with the positive reals and with the points $E_1, \ldots, E_n$ removed. Let E have positive real and imaginary parts. By the Cauchy integral theorem,

$$f(E) - f_{\text{Born}} = \frac{1}{2\pi i} \oint_C \frac{f(E') - f_{\text{Born}}}{E' - E} \, dE'$$

where C is the contour in Fig. XI.9. Since $f(E') - f_{\text{Born}} \to 0$ as $E' \to \infty$, the part of the contour marked C_0 makes no contribution as we move it out toward infinity. Thus

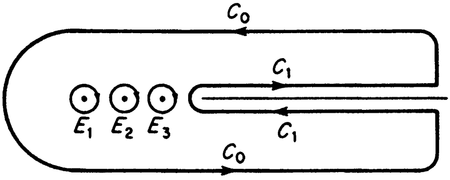


FIGURE XI.9 A contour of integration.

$$f(E) = f_{\text{Born}} + \frac{1}{2\pi i} \oint_{C_1} \frac{f(E') - f_{\text{Born}}}{E' - E} \, dE' + \sum_{j=1}^n \frac{2r_j}{E_j - E}$$

Fix E_0 on the real axis, let $E = E_0 + i\varepsilon$ and let $\varepsilon \downarrow 0$. Using $\lim_{\varepsilon \downarrow 0} (x - E_0 - i\varepsilon)^{-1} = \mathscr{P}(x - E_0)^{-1} + i\pi\delta(x - E_0)$, see (V.4), (103) results. ▌

(103) is called a **forward dispersion relation.** One of the intriguing aspects of forward dispersion relations and of the analyticity of τ_F is the connection exhibited between scattering and bound states. In particular, if we measure $f(E)$, the forward scattering amplitude, we can determine the bound state energies (or at least those with $r_j \neq 0$) by using (103). This connection between scattering and bound states will be further exhibited in Levinson's theorem (Theorem XI.59).

Our discussion of more general analyticity will require that the potential V fall off exponentially in the sense that $Ve^{\alpha|x|} \in L^1 \cap R$ for some $\alpha > 0$. For simplicity, we shall also suppose that V is spherically symmetric. In that case, the function $T(\mathbf{k}, \mathbf{k}')$ depends only on the two variables $E = k^2$ and $\cos\theta = \mathbf{k}\cdot\mathbf{k}'/E$ in the region $F \cap \{\langle \mathbf{k}, \mathbf{k}' | k = k'\rangle$. Alternatively, one often uses the variable Δ given by $\Delta^2 \equiv \frac{1}{4}(\mathbf{k} - \mathbf{k}')^2 = \frac{1}{2}E(1 - \cos\theta)$. The "physical" regions in the variables $\langle E, \cos\theta\rangle$ or $\langle E, \Delta\rangle$ are the images of $\{\langle \mathbf{k}, \mathbf{k}'\rangle \in \mathbb{R}^6 \,|\, k = k'\}$; explicitly, $\{\langle E, \cos\theta\rangle \,|\, 0 \le E < \infty;\ -1 \le \cos\theta \le 1\}$ and $\{\langle E, \Delta\rangle \,|\, 0 \le E < \infty,\ 0 \le \Delta \le \sqrt{E}\}$. It is also useful to consider the Born term

$$f_B(\Delta) = -(4\pi)^{-1} \int e^{-2i\Delta \mathbf{e}\cdot\mathbf{x}} V(x)\, d\mathbf{x}$$

For any fixed unit vector $\mathbf{e}$, $f_B(\Delta)$ is independent of $\mathbf{e}$. If $Ve^{\alpha|x|} \in L^1$, then $f_B(\Delta)$ is analytic in the region $|\mathrm{Im}\,\Delta| < \frac{1}{2}\alpha$. The general analyticity result is:

Theorem XI.47 Suppose that $Ve^{\alpha|x|} \in R$ for some $\alpha > 0$. Let $f(k, \Delta)$ be the scattering amplitude defined in the region $G \equiv \{\langle k, \Delta\rangle \,|\, k \ge 0,\ k^2 \notin \mathscr{E},\ 0 \le \Delta \le k^2\}$. Let $0 < \beta \le \alpha$ and let

$$D_\beta = \left\{\langle k, \Delta\rangle \in \mathbb{C}^2 \,\middle|\, |\mathrm{Im}\,\Delta| < \beta,\ 4\,\mathrm{Im}\,k > \alpha - \beta,\right.$$

$$\left. |\mathrm{Im}\sqrt{k^2 - \Delta^2}\,| - |\mathrm{Im}\,k| < \sqrt{\alpha^2 - (\mathrm{Im}\,\Delta)^2}\right\}$$

and let $D = \bigcup_{0 < \beta \le \alpha} D_\beta$. Then there exists a function $g(k, \Delta)$, meromorphic in D, such that if $\langle k, \Delta\rangle \in G$, then $G(k, \Delta) = f(k, \Delta) - f_{\mathrm{born}}(\Delta)$. Moreover, g has no poles in $D \cap \{\langle k, \Delta\rangle \,|\, k \in \mathbb{R}\}$ and the only poles in $D \cap \{\langle k, \Delta\rangle \,|\, \mathrm{Im}\,k > 0\}$ occur at points k where k^2 is an eigenvalue of $H_0 + V$. In particular:

(a) $f(k, \Delta)$ has an analytic continuation to a neighborhood of the physical region, and the exceptional points $\mathscr{E}$ are removable singularities.

(b) Let $h(k, z)$ be g in the new variable $z = 1 - 2k^{-2}\Delta^2$, so that $z = \cos\theta$ in the physical region. Then, for fixed k, $h(k, z)$ is analytic in the ellipse centered at $z = 0$ with foci at $z = \pm 1$, and with semimajor axis $1 + 2k^{-2}\alpha^2$. This is called the **Lehmann ellipse**.

For a proof, the reader can consult the reference given in the Notes. The main idea, already used in the proof of Theorem XI.46, is the definition of a suitably modified Lippmann–Schwinger equation. To prove that the exceptional set $\mathscr{E}$ is removable, one uses unitarity and the partial wave expansion discussed in the next section. Because the Lehmann ellipse will be used in the next section, let us show that it lies in D. Fix k real. Then $\langle k, \Delta \rangle \in D$ if and only if $(\operatorname{Im} \Delta)^2 + (\operatorname{Im} \sqrt{k^2 - \Delta^2})^2 < \alpha^2$. But $\Delta = k\sqrt{\tfrac{1}{2}(1-z)}$ and $\sqrt{k^2 - \Delta^2} = k\sqrt{\tfrac{1}{2}(1+z)}$. Thus $\langle k, \Delta \rangle \in D$ if and only if

$$(\operatorname{Im} \sqrt{1-z})^2 + (\operatorname{Im} \sqrt{1+z})^2 < 2\alpha^2/k^2$$

Since $|w|^2 = \operatorname{Re}(w^2) + 2(\operatorname{Im} w)^2$, we see that this is equivalent to

$$\begin{aligned} |1-z| + |1+z| &< 4\alpha^2 k^{-2} + \operatorname{Re}(1-z) + \operatorname{Re}(1+z) \\ &= 2(1 + 2\alpha^2 k^{-2}) \end{aligned}$$

This is precisely the ellipse in question.

Finally, we describe the strong analyticity results which hold for potentials of a special form:

Definition A **generalized Yukawa potential** is a spherically symmetric function on $\mathbb{R}^3$ of the form

$$V(r) = \sum_{j=0}^{N} r^{j-1} \int_{\mu_0}^{\infty} e^{-\mu r} \, d\rho_j(\mu)$$

where $\mu_0 > 0$, N is a finite integer, and $\rho_0, \ldots, \rho_N$ are real (but not necessarily positive) measures of finite total variation.

These potentials are "superpositions" of the basic **Yukawa potential** $r^{-1}e^{-\mu r}$ for notice that $V(r) = y^{-1} \int_{\mu_0}^{\infty} e^{-\mu r} T(\mu) \, d\mu$ where T is the distribution $T = \sum_{j=0}^{N} D^j \rho_j$. Generalized Yukawa potentials have several basic properties: (i) Since $r|V(r)| \le e^{-\mu r} \sum_{j=0}^{N} \|\rho_j\| r^j$ is bounded by $Ce^{-\frac{1}{2}\mu_0 r}$, V is in $L^2(\mathbb{R}^3)$. Thus $-\Delta + V$ is self-adjoint on $D(-\Delta)$. (ii) V falls off exponentially, so Theorem XI.47 is applicable. (iii) $V(r)$ has an analytic continuation to the region $\{r \mid |\arg r| < \tfrac{1}{2}\pi\}$ and for any real θ with $|\theta| < \tfrac{1}{2}\pi$, $V_\theta(r) \equiv V(e^{i\theta} r)$ is in L^2. This last property will play an important role in Sections XI.8 and XIII.10. It is also important in the proof of the following analyticity result:

Theorem XI.48 Let $f(k, \Delta)$ be the scattering amplitude associated with a generalized Yukawa potential. Fix k real. Then $f(k, \Delta)$ has an analytic continuation to the region of the $z(= \cos \theta)$-plane $\{z \mid z \notin [\zeta(k), \infty)\}$ where $\zeta(k) = 1 + 2k^{-2}\mu_0^2$.

This analyticity is one of several properties of f that we discuss in the Notes.

XI.8 Quantum scattering V: Central potentials

In this section we discuss some aspects of the two-body case when the potential is spherically symmetric, that is, a function only of $|x|$. Such potentials are called **central potentials**. The material that we present primarily involves the additional structure present in the central case. However, we remark that many results of the scattering theory we have already developed and of the spectral theory of Chapter XIII can be more easily proved and generalized in the central case; see for example Theorem XI.31 and Appendix 3 to this section. In the Notes to this section, we present a guide to the literature on these aspects of central potentials.

Because the subjects that we discuss are quite distinct, the section is divided into six parts: (A) We discuss the reduction of the S-operator due to symmetries. (B) This will lead us to a formal partial wave expansion of the scattering amplitude $f(E, \theta)$. Using analyticity in the Lehmann ellipse, we shall prove that the partial wave expansion converges *uniformly* when $Ve^{\alpha|x|} \in R$ for some $\alpha > 0$. (C) We shall relate the partial wave amplitudes to a quantity, called the phase shift, defined by the time-independent radial Schrödinger equation. (D) We study a nonlinear first order differential equation which yields the s-wave phase shift. (E) We develop the Jost function method of discussing the s-wave partial wave amplitude, and, in particular, we shall prove Levinson's theorem which relates the number of bound states to scattering data. (F) When V is a generalized Yukawa potential, we study the analyticity properties of the s-wave amplitude.

Except for a brief discussion in the Notes, we shall not treat continuation in angular momentum and Regge theory. In many ways, the central theorem of the section is Theorem XI.54. Some important properties of certain special functions are collected in Appendix 1. Jost functions for certain oscillatory potentials are studied in Appendix 2.

A. Reduction of the S-matrix by symmetries

We begin with the N-body case and then specialize to the two-body case. We already know that the S-operator commutes with the free energy H_0 (by a proposition preceding Theorem XI.33). If V is a central potential, then both H and H_0 commute with rotations. Thus the wave operators $\Omega^{\pm}$ and therefore the S-operator commute with rotations. In order to summarize, we make a technical definition, expressing the "natural" action of rotations on the asymptotic Hilbert space, $\mathscr{H}_{\text{asym}}$ of Section 5.

Definition Let $\mathscr{C}$ be a listing of all channels of an N-body quantum system with the proviso on degenerate eigenvalues. Fix a cluster decomposition D and an energy E and let $\mathscr{C}_1 \subset \mathscr{C}$ be the family of channels, with $D(\alpha) = D$ and $E(\alpha) = E$. Thus a channel $\alpha \in \mathscr{C}_1$ has the form

$$\alpha = \begin{pmatrix} C_1 & \cdots & C_k \\ \eta_1^{(i_1)} & \cdots & \eta_k^{(i_k)} \end{pmatrix}$$

where $\{\eta_\ell^{(i_\ell)}\}_{i_\ell}$ for ℓ fixed is an orthonormal family. Given α, $\beta \in \mathscr{C}_1$ let $J_{\beta\alpha} : \mathscr{H}_\alpha \to \mathscr{H}_\beta$ be the natural identification. Given $R \in SO(3)$, the group of three-dimensional rotations, and a function η, let $\eta \circ R^{-1}$ denote the function $(\eta \circ R^{-1})(x) = \eta(R^{-1}x)$. Since the clustered channel Hamiltonians commute with rotations, each $\eta_\ell^{(i_\ell)}$ composed with R is a linear combination

$$\eta_\ell^{(i_\ell)} \circ R^{-1} = \sum_j D_\ell^{(i_\ell, j_\ell)}(R)\eta_\ell^{(j_\ell)}$$

of the other $\eta_\ell^{(j_\ell)}$. Let $V_\alpha(R)$ denote the natural action of the rotations on $\mathscr{H}_\alpha \equiv L^2(\mathbb{R}^{3k-3})$. Then define $U_R^{(\alpha)}: \mathscr{H}_\alpha \to \bigoplus_{\beta \in \mathscr{C}_1} \mathscr{H}_\beta$ by

$$U_R^{(\alpha)} = \sum_{j_1, \ldots, j_k} \left(\prod_{\ell=1}^{k} D^{(i_\ell, j_\ell)}(R) \right) J_{\beta\alpha} V_\alpha(R)$$

where β is the channel

$$\beta = \begin{pmatrix} C_1 & \cdots & C_k \\ \eta_1^{(j_1)} & \cdots & \eta_k^{(j_k)} \end{pmatrix}$$

Finally, U_R is defined from $\bigoplus_{\alpha \in \mathscr{C}} \mathscr{H}_\alpha \to \bigoplus_{\alpha \in \mathscr{C}} \mathscr{H}_\alpha$ by $U_R \restriction \mathscr{H}_\alpha \equiv U_R^{(\alpha)}$.

Proposition 1 Let S be the S-operator of an N-body quantum system satisfying the hypotheses of Theorem XI.34 with center of mass removed. Then S commutes with $\exp(itH_{\text{asym}})$ for all $t \in \mathbb{R}$. If all the V_{ij} are central, then S commutes with all rotations, that is, $SU_R = U_R S$ for all $R \in SO(3)$.

In the classical case, we saw that symmetries considerably simplified the S-operator; a priori, the classical S-matrix was a map from $\mathbb{R}^6$ to $\mathbb{R}^6$. By using symmetries, we were able to describe S as a function from $\mathbb{R}_+ \times \mathbb{R}_+$ to $\mathbb{R} \times [0, \pi]$. We shall find the restrictions that symmetries place on the quantum-mechanical S-operator. First we study the effect of energy conservation by giving a general proposition about operators commuting with a one-parameter group.

Definition Let $\langle M, \mu \rangle$ be a σ-finite measure space, let $\mathscr{H}_0$ be a separable Hilbert space, and let $\mathscr{H} = L^2(M, d\mu; \mathscr{H}_0)$. We say that a function a from M to $\mathscr{L}(\mathscr{H}_0)$, the bounded operators on $\mathscr{H}_0$, is *measurable* if $(\psi, a(\cdot)\varphi)$ is measurable for each ψ, $\varphi \in \mathscr{H}_0$. We say that $a \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}_0))$ if a is measurable and ess.sup. $\|a(\cdot)\|_{\mathscr{L}(\mathscr{H}_0)} < \infty$. Given $a \in L^\infty(M, d\mu; \mathscr{L}(\mathscr{H}_0))$, there is, by the Riesz lemma, an operator $A \in \mathscr{L}(\mathscr{H})$ so that for each ψ, $\varphi \in \mathscr{H}$,

$$(\psi, A\varphi)_{\mathscr{H}} = \int_M (\psi(\lambda), a(\lambda)\varphi(\lambda))_{\mathscr{H}_0} \, d\mu(\lambda)$$

We call such a map a **decomposable operator** and call $a(\lambda)$ **the fiber of A at λ**. A determines its fibers a.e.

Fibered operators are further discussed in Section XIII.16 where the Riesz lemma argument occurs as part of Theorem XIII.83.

Proposition 2 Let $\mathscr{H}_0$ be a separable Hilbert space and let μ be a Borel measure on $\mathbb{R}$. Let B be multiplication by x on $L^2(\mathbb{R}, d\mu; \mathscr{H}_0) \equiv \mathscr{H}$. Suppose that $A \in \mathscr{L}(\mathscr{H})$ commutes with e^{itB} for each $t \in \mathbb{R}$. Then A is a decomposable operator. Moreover, if A is unitary (respectively, self-adjoint), then its fibers are (a.e.) unitary (respectively, self-adjoint) operators on $\mathscr{H}_0$.

The first part of the proposition is a special case of Theorem XIII.84. The second part is easy since A and its fibers are bounded.

Example 1 Let S be the S-matrix for scattering from a reduced two-body system of reduced mass $\frac{1}{2}$ on $L^2(\mathbb{R}^m) = \mathscr{H}$. Suppose that S is unitary. Let $\mathscr{H}_0$ be the Hilbert space $L^2(S^{m-1}; d\Omega)$ where S^{m-1} is the unit sphere in $\mathbb{R}^m$ and $d\Omega$ is its standard surface measure. Define the unitary map $U: L^2(\mathbb{R}^m) \to L^2(\mathbb{R}_+, dE; \mathscr{H}_0)$ by

$$[(Uf)(E)](\omega) = (\sqrt{2})^{-1} E^{(m-2)/4} \hat{f}(E^{1/2}\omega) \tag{104}$$

where $\omega \in S^{m-1}$ is viewed as a unit vector in $\mathbb{R}^m$. When we are given an operator A on $L^2(\mathbb{R}^m)$, we shall call UAU^{-1} "the operator A in the energy representation." In the energy representation, H_0 is multiplication by E, so that Proposition 2 above is applicable to S by Proposition 1. Thus, in the energy representation, S is a decomposable operator whose fibers $S(E)$ are unitary maps of $L^2(S^{m-1}, d\Omega)$ to itself. We define $T(E)$ by

$$T(E) = (2\pi i)^{-1}(I - S(E))$$

In case $m = 3$ and $V \in L^1 \cap R$, Theorem XI.42 provides an explicit representation for $T(E)$, namely

$$(T(E)f)(\omega) = \frac{E^{1/2}}{2} \int_{S^{m-1}} T(E^{1/2}\omega, E^{1/2}\omega') f(\omega')\, d\Omega(\omega') \tag{105}$$

where $T(\cdot, \cdot)$ is the "T-matrix." We shall pursue this realization of $T(E)$ as an integral operator below.

Example 2 Let $\mathscr{H}_{\text{asym}}$ be the asymptotic Hilbert space for an N-body quantum system on $L^2(\mathbb{R}^{3N-3})$. Recall that for each $\alpha \in \mathscr{C}$, an index set for the channels, we defined the channel energy E_α to be the sum of the internal energy of the clusters in α. E_α is sometimes called the **threshold for channel α**. For each $E \in \mathbb{R}$, the set

$$\mathscr{C}_E = \{\alpha \in \mathscr{C} \mid E_\alpha < E\}$$

is called the **set of open channels** at energy E. Let α be an ℓ-cluster channel so that the channel Hilbert space $\mathscr{H}_\alpha = L^2(\mathbb{R}^{3\ell-3})$. As in the two-body case (Example 1), we can realize H_α as multiplication by $(E + E_\alpha)$ on $L^2(\mathbb{R}_+, dE; L^2(S^{3\ell-4}, d\mu_\alpha))$ although μ_α and the explicit formula for the energy representation are more complicated than (104) because of the possible different masses of different clusters. Next suppose that one can write $[E, \infty) = \bigcup_{n=1}^\infty I_n$ where: (1) $E = \inf \sigma(H)$; (2) the I_n are disjoint intervals; (3) for each fixed n, the set $\mathscr{C}_E$ is the same for each $E \in I_n$. Such a decomposition exists so long as H has "reasonable" spectral properties, for example, if each subsystem has $\sigma_{\text{pp}}(H(C)) = \sigma_{\text{disc}}(H(C))$ or if each $H(C)$ has eigenvalues that cluster only at thresholds (Problem 74); in Section XIII.10 we shall see that such spectral properties can sometimes be proven. Let $\{P_\Omega\}$ be the spectral projections for H_{asym} and write $\mathscr{H}_{\text{asym}} = \bigoplus_{n=1}^\infty \mathscr{H}^{(n)}$ where $\mathscr{H}^{(n)} = \text{Ran } P_{I_n}$. Since S commutes with each P_Ω, it leaves each $\mathscr{H}^{(n)}$ invariant. It is now possible to apply Proposition 2 and obtain a fibering of each $S \restriction \mathscr{H}^{(n)}$. One can think of S itself as a generalized decomposable operator, but the fibers $S(E)$ are maps on Hilbert spaces with some E dependence; explicitly $S(E)$ is a map on $\mathscr{H}_E \equiv \bigoplus_{\alpha \in \mathscr{C}_E} \mathscr{H}_\alpha^{(0)}$ where $\mathscr{H}_\alpha^{(0)} = L^2(S^{3\ell-4}, d\mu_\alpha)$. As E is increased, the Hilbert space $\mathscr{H}_E$ on which the fibers act increases each time a new scattering threshold is passed. We remark that the energy representation we have just described where the space $\mathscr{H}_E$ is not independent of E is discussed most naturally in the language of direct integrals of Hilbert spaces.

Before turning to the consequences of rotational invariance, we want to study the operators $T(E)$ of Example 1 in more detail:

Theorem XI.49 Let $H = -\Delta + V$ where V is in R. Then:

(a) For each $E \in \mathbb{R}_+ \backslash \mathscr{E}$, the map $T(E)$ on $L^2(S^2, d\Omega)$ is Hilbert–Schmidt.
(b) $E \to T(E)$ is a continuous map from $\mathbb{R}_+ \backslash \mathscr{E}$ to the Hilbert–Schmidt operators with their natural topology.
(c) As $E \to \infty$, $T(E) \to 0$ in operator norm.

If, moreover, V is in L^1, then "Hilbert–Schmidt" in (a) and (b) can be replaced with "trace class."

Proof For each $E > 0$, let $K_V(E)$ be the Hilbert–Schmidt operator on $L^2(\mathbb{R}^3)$ with kernel.

$$\frac{|V(x)|^{1/2} e^{i\sqrt{E}|x-y|} V(y)^{1/2}}{4\pi |x-y|}$$

and let $F_V(E)$ be the map from $L^2(\mathbb{R}^3)$ to $L^2(S^2, d\Omega)$ given by

$$(F_V(E)f)(\omega) = \tfrac{1}{4} E^{1/4} \pi^{-3/2} \int \exp(-iE^{1/2}\omega \cdot x) V^{1/2}(x) f(x)\, dx \quad (106)$$

Our main tool will be to show that $F_V(E)$ is a bounded operator in the class $\mathscr{I}_4$ (defined in the Appendix to Section IX.4) and that

$$T(E) = F_V(E)[I + K_V(E)]^{-1} F_{|V|}(E)^* \quad (107)$$

for all $E \in \mathbb{R}_+ \backslash \mathscr{E}$. (107) is intimately related to (99). We shall need the formula

$$(F_V(E)^* g)(x) = \tfrac{1}{4} E^{1/4} \pi^{-3/2} \int \exp(+iE^{1/2}\omega \cdot x) V^{1/2}(x) g(\omega)\, d\Omega(\omega) \quad (108)$$

Suppose first that $V \in L^1 \cap R$. Then $T(E)$ is given as the integral operator (105) with

$$T(k, k') = (2\pi)^{-3} \int V(x)^{1/2} e^{-ik \cdot x} \psi(x, k')\, dx$$

where

$$\psi(\cdot, k) = [I + K_V(k^2)]^{-1} \psi_0(\cdot, k)$$

and

$$\psi_0(x, k) = |V(x)|^{1/2} \exp(ik \cdot x)$$

As a result, (107) is proven in this case.

We next need the following properties of $F_V(E)$ whose proofs are left to the reader (Problem 75):

(1) When $V \in R$, $F_V(E) \in \mathscr{I}_4$, that is, $F_V(E)^*F_V(E)$ is Hilbert–Schmidt.
(2) $E \to F_V(E)$ is continuous in the $\mathscr{I}_4$ topology.
(3) For fixed $E \neq 0$, $V \to F_V(E)$ is continuous from the class of Rollnik potentials with their natural norm to $\mathscr{I}_4$.

(1′)–(3′) If R is replaced by $L^1 \cap R$ and $\mathscr{I}_4$ by $\mathscr{I}_2$, (1)–(3) still hold.

For example, the explicit formula (106) shows that $F_V(E)$ has an L^2 kernel when $V \in L^1$ (proving (1′)) and the explicit formula

$$(F_V(E)^*F_V(E)g)(x) = \int \frac{V(x)^{\frac{1}{2}}V(y)^{\frac{1}{2}}}{|x-y|4\pi^2} \sin(E^{1/2}|x-y|)g(y)\,dy$$

proves (1).

In addition, we need a fact which is proven by combining the theory of smooth perturbations with the Kato–Birman theory (see Problem 57 of Chapter XIII):

(4) If $V_n \to V$ in Rollnik norm, then the corresponding S-matrices converge strongly.

Fix $V \in R$ and choose $V_n \in L^1 \cap R$ so that $V_n \to V$ in Rollnik norm. Suppose that $E_0 \in \mathbb{R}_+ \backslash \mathscr{E}$. Since we can find an interval A about E_0 so that $\bar{A} \cap \mathscr{E} = \emptyset$ and since the map $\langle V, E\rangle \mapsto K_V(E)$ of $R \times \mathbb{R}_+$ into $\mathscr{I}_2$ is jointly continuous (Problem 76), for all large n, A is disjoint from the exceptional set $\mathscr{E}_n$ for $-\Delta + V_n$. Since the S-matrices S_n converge to S (by (4)), since $F_{V_n}(E) \to F_V(E)$ (by (3)), and since we know that (107) holds for each V_n, it holds for V as long as $E \in A$. (a) and (b) now follow from (2) and (107). The proof of (c) is left to the reader (Problem 77). ▮

Using the method of weighted L^2 estimates (Section XIII.8), (107) and certain continuity properties of $T(E)$ can be extended to potentials behaving like $r^{-1-\varepsilon}$ at infinity (see the references in the Notes to Section XIII.8).

Since $T(E)$ is a Hilbert–Schmidt operator, it has an integral kernel $t(E; \omega, \omega')$. Because of a difference in normalization, t should be distinguished from the T-matrix T of Section 6; in fact, as we have seen (105):

$$t(E; \omega, \omega') = \tfrac{1}{2}E^{1/2}T(E^{1/2}\omega, E^{1/2}\omega')$$

when $V \in L^1 \cap R$. Unfortunately, this distinction between t and T is typical of obnoxious factors of $E^{1/2}$, 2π, -1, and i which continually crop up in scattering theory.

Suppose now that V is a central potential. Since S commutes with rotations, so does $T(E)$ for almost all E. Because $E \to T(E)$ is continuous on

$\mathbb{R}_+ \backslash \mathscr{E}$, we conclude that $T(E)$ commutes with rotations. Thus for every rotation R acting on S^2 and $E \in \mathbb{R}_+ \backslash \mathscr{E}$,

$$t(E; R\omega, R\omega') = t(E; \omega, \omega')$$

It follows that $t(E; \omega, \omega')$ is a function only of $\omega \cdot \omega' \equiv \cos\theta$. We state our final result in terms of the quantity f of (96) and (97), which is related to the differential cross section by $d\sigma/d\Omega = |f|^2$.

Definition $f(E, \cos\theta) = -(2\pi)^2 E^{-1/2} t(E; \omega, \omega')$ where $\omega \cdot \omega' = \cos\theta$. f is called the **scattering amplitude**.

We summarize the reduction due to symmetrics:

Theorem XI.50 Let $V \in R$ be a central potential and let S be the S-operator for $-\Delta + V$. Then there is a function $f(E, \cos\theta)$ from $(\mathbb{R}_+ \backslash \mathscr{E}) \times [-1, 1]$ to $\mathbb{C}$ so that the fibers of S, $S(E)$, have integral kernel:

$$(S(E) - I)(\omega, \omega') = \frac{i}{2\pi} E^{1/2} f(E, \omega \cdot \omega')$$

Thus the classical reduced S-function from $\mathbb{R}_+ \times \mathbb{R}_+$ to $\mathbb{R} \times [0, \pi]$ is replaced with a single *complex-valued* function on $\mathbb{R}_+ \times [0, \pi]$. If we separate f into its argument and magnitude, we obtain two real-valued functions. Since the scattering cross section depends only on the magnitude of f, this magnitude is the analogue of the classical scattering angle function in that it contains the same kind of physical information. In a sense which can be made precise, the argument of f contains time-delay information (see the references in the Notes).

B. The partial wave expansion and its convergence

We have just seen that $T(E)$ is a Hilbert–Schmidt operator. It is also normal because $S(E)$ is unitary. Thus $T(E)$ has a complete orthonormal set of eigenvectors. As a result, so does $S(E)$. If the potentials are central, we can identify the eigenvectors by using the rotational invariance! The group $SO(3)$ of rotations acting on $L^2(S^2, d\Omega)$ induces a decomposition of $L^2(S^2, d\Omega)$ into a direct sum $\oplus_{\ell=0}^{\infty} \mathscr{H}_\ell$ where $\mathscr{H}_\ell$ is the $(2\ell + 1)$-dimensional subspace spanned by the spherical harmonics of order ℓ. Each subspace is left invariant by $SO(3)$ and the restriction of the action of $SO(3)$ to $\mathscr{H}_\ell$ is an irreducible representation (see Section XVI.2 for the basic definitions and for Schur's lemma). The representations are inequivalent for distinct ℓ. It follows by Schur's lemma that $S(E)$ leaves each $\mathscr{H}_\ell$ invariant and that there exist numbers $s_\ell(E)$ so that for each $\psi \in \mathscr{H}_\ell$,

$$S(E)\psi = s_\ell(E)\psi$$

Definition The quantities $s_\ell(E)$ are called **partial wave S-matrix elements.** The quantities $f_\ell(E)$ defined by

$$f_\ell(E) = (2iE^{1/2})^{-1}[s_\ell(E) - 1] \tag{109}$$

are called **partial wave scattering amplitudes.**

Theorem XI.51 (partial wave expansion: L^2 convergence theorem) Let $V \in R$ be a central potential and fix $E \in \mathbb{R}_+ \backslash \mathscr{E}$. Then the partial wave amplitudes $f_\ell(E)$ and the scattering amplitude $f(E, \cos\theta)$ are related by

$$f(E, \cos\theta) = \sum_{\ell=0}^{\infty} (2\ell + 1) f_\ell(E) P_\ell(\cos\theta) \tag{110a}$$

$$f_\ell(E) = \tfrac{1}{2} \int_{-1}^{1} f(E, z) P_\ell(z)\, dz \tag{110b}$$

The sum in (110a) is convergent to $f(E, \cos\theta)$ in $L^2(S^2, d\Omega)$-norm for each fixed E. (110a) is called the **partial wave expansion.** The functions $P_\ell(z)$ are the Legendre polynomials. We summarize their properties in an appendix to this section.

Proof Let ω_0 be a fixed direction. Then $P_\ell(\omega \cdot \omega_0)$ is an element of the subspace $\mathscr{H}_\ell$, so

$$\int t(E; \omega, \omega') P_\ell(\omega' \cdot \omega_0)\, d\Omega(\omega') = (-2\pi i)^{-1}(s_\ell(E) - 1) P_\ell(\omega \cdot \omega_0)$$

Picking $\omega = \omega_0$ and using the formula defining $f(E; \omega \cdot \omega')$, we see that

$$\int f(E; \omega' \cdot \omega_0) P_\ell(\omega' \cdot \omega_0)\, d\Omega(\omega') = 4\pi f_\ell(E) P_\ell(1)$$

Since $P_\ell(1) = 1$ and $\int f(\omega')\, d\Omega(\omega') = 2\pi \int f(\omega')\, d(\omega' \cdot \omega_0)$ for functions f of $\omega' \cdot \omega_0$, (110b) results. On the other hand, since $t(E; \omega, \omega')$ is the kernel of a Hilbert–Schmidt operator, $\int_{-1}^{1} |f(E; z)|^2\, dz < \infty$. Since the $P_\ell(z)$ are a complete orthogonal family with $\int_{-1}^{1} |P_\ell(z)|^2\, dz = 2(2\ell + 1)^{-1}$, (110a) follows from (110b). ∎

The orthogonality relations for the P_ℓ functions have an important consequence. For, the total cross section is given by $\sigma = \int (d\sigma/d\Omega)\, d\Omega = 2\pi \int_{-1}^{1} |f(E; z)|^2\, dz$, so we obtain the basic formula

$$\sigma(E) = 4\pi \sum_{\ell=0}^{\infty} (2\ell + 1)|f_\ell(E)|^2 \tag{111}$$

It is sometimes possible to make a much stronger statement about the convergence of the partial wave expansion than we have in Theorem XI.51:

Theorem XI.52 (partial wave expansion; uniform convergence theorem) Let V be a central potential with $e^{\alpha|x|}V \in R$ for some $\alpha > 0$. Fix $E \in \mathbb{R}_+ \backslash \mathscr{E}$. Then the partial wave expansion (110a) converges uniformly for $\theta \in [0, 2\pi]$.

Proof By Theorem XI.47, $f(E, z)$ is analytic for z in the ellipse with foci ± 1 and semimajor axis $1 + 2\alpha^2 E^{-1}$. The uniform convergence of the partial wave expansion on compact subsets of this ellipse now follows from a general theorem on the convergence of Legendre series (Theorem XI.63 in Appendix 1). ▌

C. Phase shifts and their connection to the Schrödinger equation

In part B we did not make use of the fact that the S-matrix is unitary. This fact immediately implies that the numbers $s_\ell(E)$, which are eigenvalues of $S(E)$, have modulus one.

Definition The **phase shifts** $\delta_\ell(E)$, are defined by the equation

$$s_\ell(E) = e^{2i\delta_\ell(E)}$$

A priori, the phase shifts are real numbers defined for almost every E, and they are only determined modulo π. Let $E_0 = \max\{E \mid E \in \mathscr{E}\}$ where $\mathscr{E}$ is the exceptional set. Since $\lim_{E\to\infty} S(E) = I$ and $S(E)$ is continuous on (E_0, ∞), we can eliminate the a.e. and modulo π ambiguities for $E \in (E_0, \infty)$ by requiring that $\delta_\ell(E)$ be continuous there and that $\lim_{E\to\infty} \delta_\ell(E) = 0$. Under mild assumptions, we shall see in Sections D and E below that $s_0(E)$ and hence $\delta_0(E)$ can be chosen to be continuous on $[0, \infty)$. Similarly, one can also prove that $\delta_\ell(E)$ can be chosen continuous for $\ell > 0$. The phase shift, defined to be continuous in E and to obey $\lim_{E\to\infty} \delta_\ell(E) = 0$ for each fixed ℓ, also obeys $\lim_{\ell\to\infty}\delta_\ell(E)=0$ for each fixed E. In fact, since $S(E)-I$ is Hilbert–Schmidt when $V\in R$, one has $\sum_{\ell=0}^{\infty}(2\ell+1)|\delta_\ell(E)|^2<\infty$ in that case.

The partial wave amplitude can now be written in three different ways, each of them useful in different contexts:

$$f_\ell(E)=(2ik)^{-1}(e^{2i\delta_\ell(E)}-1) \tag{112a}$$

$$f_\ell(E)=k^{-1}e^{i\delta_\ell(E)}\sin\delta_\ell(E) \tag{112b}$$

$$f_\ell(E)=k^{-1}(\cot\delta_\ell(E)-i)^{-1} \tag{112c}$$

where $k=\sqrt{E}$. In the rest of this section k will always denote $\sqrt{E}$. Notice that (112b) implies that

$$\operatorname{Im} f_\ell(E)=k\,|f_\ell(E)|^2 \tag{113}$$

This is often called **partial wave unitarity** because it is a direct translation of the unitarity of S. (110), (111), and (113) yield a new proof of the unitarity relation (97c).

The most important tool in the scattering theory for central potentials is the connection between phase shifts and the time-independent radial Schrödinger equation given by:

Theorem XI.53 Let V be central and piecewise continuous as a function of r on $[0,\infty)$. Suppose that $\int_0^1 r|V(r)|\,dr$ and $\int_1^\infty |V(r)|\,dr$ are finite. Fix $E>0$ and a nonnegative integer ℓ. Then there exists a unique function $\varphi_{\ell,E}(r)$ on $(0,\infty)$ that is C^1 and piecewise C^2 and which satisfies the equation

$$-\varphi''(r)+V_\ell(r)\varphi(r)=E\varphi(r) \tag{114}$$

where

$$V_\ell(r)=V(r)+\ell(\ell+1)r^{-2}$$

together with the boundary conditions

$$\lim_{r\to0}\varphi_{\ell,E}(r)=0,\qquad \lim_{r\to0}r^{-\ell-1}\varphi_{\ell,E}(r)=1$$

Further, there exists a constant c so that

$$\lim_{r\to\infty}\left[c\varphi_{\ell,E}(r)-\sin(kr-\tfrac{1}{2}\pi\ell+\delta_\ell(E))\right]=0 \tag{115}$$

where $\delta_\ell(E)$ is the scattering phase shift.

Proof One part of the proof involves applying the theory of ordinary differential equations to study (114). We shall quote several results of this study without proof. Later, in Section E, we shall prove these results in the case $\ell = 0$. For proofs of the general ℓ results, see the references in the Notes. Although the second boundary condition implies the first, we write down both to emphasize the parallel to a second-order equation with $\varphi(x_0) = a$ and $\varphi'(x_0) = b$ as boundary conditions.

First suppose that $V \in C_0^\infty(\mathbb{R}^3)$ and that V is central. Fix a direction $\mathbf{e}$ and let $\varphi(\mathbf{x}, k\mathbf{e})$ be the Lippmann–Schwinger wave function constructed in the proof of Theorem XI.41. Then

$$\varphi(x, ke) = e^{ike \cdot x} - \frac{1}{4\pi} \int \frac{e^{ik|x-y|}}{|x-y|} V(y)\varphi(y, ke)\, dy \tag{116}$$

Let $g \in C_0^\infty$ and let $h = (-\Delta - E)g$. Then

$$\int h(x)\varphi(x, ke)\, dx = -\frac{1}{4\pi} \iint h(x) \frac{e^{ik|x-y|}}{|x-y|} V(y)\varphi(y, ke)\, dy\, dx \tag{117}$$

where we have used the fact that $(-\Delta - E)e^{ike \cdot x} = 0$ in distributional sense to eliminate the first term in (116). Since $|V|^{1/2}\varphi \in L^2$ and V and h are in C_0^∞, we can interchange the order of integration on the right-hand side of (117) and use

$$\int [(-\Delta - E)g](x) \frac{e^{ik|x-y|}}{4\pi|x-y|}\, d^3x = g(y)$$

to conclude that $(-\Delta - E)\varphi(x, ke) = -V(x)\varphi(x, ke)$ in distributional sense. By the elliptic regularity theorem (Theorem IX.26), we conclude that $\varphi(x, ke)$ is C^∞ in x and obeys the partial differential equation $(-\Delta + V)\varphi = E\varphi$ in the classical sense. Choose spherical coordinates $\langle r, \theta, \eta \rangle$ where θ is the angle between r and e. Then φ is independent of the azimuthal angle η. Let

$$\tilde{\varphi}_{\ell, E}(r) = \frac{r}{2} \int_0^\pi \varphi(r, \theta; ke) P_\ell(\cos\theta) \sin\theta\, d\theta$$

Then $\tilde{\varphi}_{\ell, E}$ obeys (114) and the first boundary condition. The theory of ordinary differential equations tells us that every solution of (114) obeying the first boundary condition is a multiple of the unique solution obeying both boundary conditions. If $\ell \neq 0$, so that V_ℓ is singular at $r = 0$, this fact is not as easy as in the case $\ell = 0$ where we can appeal to Section V.6.A.

The proof of the theorem in case $V \in C_0^\infty$ is thus reduced to proving (115) with $\tilde{\varphi}$ replacing φ. In (116) fix $x \cdot e/|x|$ and let $|x| \to \infty$. Using the definition of $T(\mathbf{k}, \mathbf{k}')$ and the fact that $V\varphi$ has compact support, it is easy to show that (Problem 78):

$$\lim_{\substack{|x|\to\infty \\ x\cdot e=|x|\cos\theta_0}} \left(\int \frac{e^{ik|x-y|}}{|x-y|} V(y)\varphi(y, ke)\, dy\right) e^{-ik|x|}|x| = (2\pi)^3 T(ke', ke) \tag{118}$$

where e' is chosen with $e \cdot e' = \cos\theta_0$. Moreover, the limit is uniform in θ_0. (105), (110b), and the definition of f imply that

$$\frac{1}{2}\int_0^\pi P_\ell(\cos\theta)\left[T(ke', ke)\Big|_{e\cdot e'=\cos\theta}\right]\sin\theta\, d\theta = -\frac{1}{2\pi^2} f_\ell(E)$$

By (116) and the uniformity of the limit in (118), we have

$$\lim_{r\to\infty} [\tilde{\varphi}(r) - e^{i\pi\ell/2} r j_\ell(kr) - f_\ell(E)e^{ikr}] = 0 \tag{119}$$

Here $j_\ell(kr)$ is the spherical Bessel function defined in the first appendix to this section. By Theorem XI.64, $y j_\ell(y) - \sin(y - \pi\ell/2) \to 0$ as $y \to \infty$ and moreover $f_\ell(E) = (e^{2i\delta_\ell} - 1)/2ik$. Thus

$$\lim_{r\to\infty} [2ik\tilde{\varphi}(r) - (e^{ikr} - e^{-ikr}e^{i\pi\ell}) - (e^{2i\delta_\ell} - 1)e^{ikr}] = 0$$

or

$$\lim_{r\to\infty} [ke^{-i\pi\ell/2}e^{-i\delta_\ell}\tilde{\varphi}(r) - \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell)] = 0$$

This proves the theorem when $V \in C_0^\infty$. We approximate general V by $V_n \in C_0^\infty$. By Theorem XI.31 and Problem 28, as $V_n \to V$, the corresponding S-matrices converge, so the corresponding values of δ_ℓ converge. On the other hand, the method of Section E shows that the shifts of the phase of the solution of (114) converge. ▮

Thus δ_ℓ represents the shift in the phase of the solution of the radial Schrödinger equation regular at $r = 0$ relative to $j_\ell(kr)$, the solution when $V = 0$. In the above theorem we can drop the smoothness assumption on V if we replace the differential equation (114) by the integral equation (125). It is possible to prove (115) by developing a scattering theory directly for the Schrödinger operators on a fixed angular momentum subspace. This is discussed in Appendix 3.

D. The variable phase equation

In Section C we proved that the phase shift was connected to the radial Schrödinger equation. This connection suggests a great many additional results. For example, fix V obeying the conditions of Theorem XI.53. Suppose we make V more negative somewhere. Then for each fixed k, the solutions of $-\varphi'' + V_\ell \varphi = k^2\varphi$ oscillate more rapidly in the region where V has been made more negative. Thus we expect that the phase shift should be larger. We thus see that one expects that $\delta \geq \tilde{\delta}$ if $V \leq \tilde{V}$. It turns out to be difficult to prove this directly because of the π ambiguity in δ. For this reason, it is useful to develop additional tools for studying the phase shift. We develop two different methods in this subsection and the next. Both depend ultimately on Theorem XI.53.

Theorem XI.54 Let V obey the hypotheses of Theorem XI.53. Then, for each $k > 0$, there exists a unique solution of the equation

$$d'(r) = -\frac{1}{k} V(r)\sin^2(kr + d(r)), \qquad r \in (0, \infty) \tag{120}$$

satisfying the boundary condition $\overline{\lim}_{r\to 0}\, r^{-1}|d(r)| < \infty$. Moreover, the solution satisfies

$$\lim_{r\to\infty} d(r) = \delta_{\ell=0}(k^2) \tag{121}$$

where $\delta_{\ell=0}(k^2)$ is the s-wave phase shift for V, $\delta_0(k^2)$. Equation (120) is called the **variable phase equation**. We emphasize that $d(r)$ is k-dependent.

Proof The existence of solutions with the right boundary conditions follows from the contraction mapping theorem according to the pattern discussed in Section V.6.A. We leave the proof to Problem 79.

Fix ρ in $(0, \infty)$ and let V^ρ be defined by

$$V^\rho(r) = \begin{cases} V(r), & r \leq \rho \\ 0, & r > \rho \end{cases}$$

Let δ^ρ be the phase shift for V^ρ at fixed energy k^2. Since $V^\rho \to V$ in the norm given by (61), $\delta^\rho \to \delta$ as $\rho \to \infty$ (modulo π). We shall show that the function $\rho \mapsto \delta^\rho$ obeys the differential equation and the boundary condition at 0. This will allow us to conclude that (121) holds modulo π. We leave the question of resolving the modulo π ambiguity to Problem 80.

Let φ solve (114) for $\ell = 0$ and satisfy $\lim_{r\to 0} r^{-1}\varphi(r) = 1$. Let φ^ρ be the analogous function for V^ρ. Clearly,

$$\varphi^\rho(r) = \begin{cases} \varphi(r), & r \le \rho \\ \alpha \sin(kr + \beta), & r \ge \rho \end{cases}$$

for suitable α and β. By Theorem XI.53, $\beta = \delta^\rho$. The requirement that φ^ρ be C^1 implies

$$k \cot(k\rho + \delta^\rho) = \varphi'(\rho)/\varphi(\rho) \tag{122}$$

Using (122) and the differential equation (114), it is easy to prove that (Problem 81):

$$\frac{d\delta^\rho}{d\rho} = -\frac{1}{k} V(\rho)\sin^2(k\rho + \delta^\rho) \tag{123}$$

Moreover, by (122), $\lim_{\rho\to 0} \cot(k\rho + \delta^\rho) = \infty$. We resolve the π ambiguity in δ^ρ as defined in (122) by requiring $\lim_{\rho\to 0} \delta^\rho = 0$, and that δ^ρ be C^1. Finally, by (122), $\lim_{\rho\to 0} k\rho \cot(k\rho + \delta^\rho) = 1$ or

$$\lim_{\rho\to 0} (k\rho)^{-1}(k\rho + \delta^\rho) = 1$$

so, $\lim_{\rho\to 0} \rho^{-1}\delta^\rho = 0$. Thus by the uniqueness of solutions to equation (120), $\delta^\rho = d(\rho)$. ▮

Corollary 1 $\delta_0(E)$ may be chosen continuous in E for all E.

This is a corollary of part of the proof contained in Problem 80.

Corollary 2 If $\delta_0(E)$ is chosen to be continuous with $\lim_{E\to\infty} \delta_0(E) = 0$, then the phase shifts for $-\Delta + \lambda V$ are continuous in λ and go to zero as $\lambda \to 0$.

The proof is left to Problem 82.

Corollary 3 δ_0 is positive for an everywhere negative potential ($V(r) \le 0$ all r) and negative for an everywhere positive potential.

Proof $\delta_0(k^2) = -k^{-1} \int_0^\infty V(r)\sin^2(kr + d(r))\, dr$ by (120) and (121). This is clearly positive (respectively, negative) if $V \le 0$ (respectively, $V \ge 0$). ▮

Corollary 4 If $V \le \tilde{V}$, the s-wave phase shifts for V are greater than or equal to those for $\tilde{V}$.

Proof Fix $k > 0$. Suppose first that $V = \tilde{V}$ in $(0, \rho_0)$ and that $V < \tilde{V}$ in (ρ_0, ∞). Let $d(\rho)$, $\tilde{d}(\rho)$ be the corresponding solutions of the variable phase equation, (120). Then $d(\rho_0) = \tilde{d}(\rho_0)$ and $d'(\rho_0) = \tilde{d}'(\rho_0)$ by (120), so $d(\rho) > \tilde{d}(\rho)$ for ρ near and larger than ρ_0. If $\tilde{d}$ were ever larger than d, there would be $\rho_1 > \rho_0$ with $d(\rho_1) = \tilde{d}(\rho_1)$ and $\tilde{d}'(\rho_1) \geq d'(\rho_1)$. This is inconsistent with (120) and $V < \tilde{V}$ in (ρ_0, ∞). Thus $d \geq \tilde{d}$ for all ρ and, by (121), $\delta \geq \tilde{\delta}$. For the general case, one uses a simple limiting argument. ▌

The low energy behavior of $\delta_0(E)$ is of especial interest. It may be studied by a method related to the variable phase method.

Theorem XI.55 Let $V \in C_0^\infty(\mathbb{R}^3)$ be a central potential and let u be the solution of $-u''(r) + V(r)u(r) = 0$ with boundary conditions $u(0) = 0$, $u'(0) = 1$. Then:

(a) If $\lim_{r\to\infty} u'(r) \neq 0$ and $u(r)$ has m zeros different from $r = 0$, then

$$\lim_{k\to 0} \delta_0(k^2) = m\pi \qquad \text{and} \qquad \lim_{k\to 0} \frac{\delta_0(k^2) - m\pi}{k} = \lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)}$$

(b) If $\lim_{r\to\infty} u'(r) = 0$ and $u(r)$ has m zeros different from $r = 0$, then

$$\lim_{k\to 0} \delta_0(k^2) = (m + \tfrac{1}{2})\pi$$

Proof We use equations (122) and (123). Choose R so that all the zeros of u lie in $(0, R)$ and so that $V(r) = 0$ if $r > R$. In particular, $u(r) = a(r - R) + b$ for $r > R$. Since $u(r)$ has no zeros in (R, ∞), we have that $a/b = u'(R)/u(R) \geq 0$. Let $\varphi_E(r)$ denote the solution of (114) satisfying $\varphi_E(0) = 0$ and $\varphi_E'(0) = 1$. Writing the differential equation as an integral equation, one sees that $\varphi_E(r) \to \varphi_0(r)$ as $E \to 0$, uniformly on $[0, R + 1]$. In particular, for some E_0, $\varphi_E(r)$ has m zeros in $[0, R)$ if $E < E_0$ and $\varphi_E(R)^{-1}\varphi_E'(R) \to a/b$. By the proof of Theorem XI.54, $\delta_0(E)$ is determined by

$$k \cot(k\rho + d(\rho, k)) = \varphi_E'(\rho)/\varphi_E(\rho) \tag{122}$$

$d(\cdot, k)$ continuous, $d(0, k) = 0$, $d(R, k) = \delta_0(k^2)$. Clearly at each point ρ that $\varphi_E(\rho)$ vanishes, $k\rho + d(\rho, k)$ must take one of the values $0, \pm\pi, \ldots$. Moreover, by (123), at each such point, $(\partial/\partial\rho)d(\rho, k) = 0$, so that $(\partial/\partial\rho)(k\rho + d(\rho, k)) > 0$. Thus

$$m\pi \leq kR + d(R, k) < (m + 1)\pi \tag{124}$$

if $k < E_0$. $d(R, k) = \delta_0(k)$ is thus uniquely determined by (122) and (124). If $u'(R) = \lim_{r\to\infty} u(r) \neq 0$, then for all small E, $\varphi_E'(R)/\varphi_E(R) \geq \frac{1}{2}u'(R)/u(R) > 0$

so, by (122), $\cot(kR + d(R, k)) \to \infty$ as $k \to 0$. This is only consistent with (124) if $kR + d(k, R) \to m\pi$. On the other hand, by the integral equation, $\varphi_E'(R)$ is a C^∞ function of k^2 at $k = 0$, so if $u'(R) = 0$, then $\varphi_E'(R)$ vanishes as k^2 at $k = 0$. Thus, in that case, $\cot(kR + d(R, k)) \to 0$ by (122), so $kR + d(R, k) \to (m + \frac{1}{2})\pi$. The remaining statement in (a) is left to the reader (Problem 83). ▮

It is possible to considerably weaken the hypotheses on V in the preceding theorem.

Definition The quantity

$$\lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)} = \lim_{k\to 0} \frac{\delta_0(k) - \delta_0(0)}{k}$$

is called the **scattering length.** If $\lim_{r\to\infty} u'(r) = 0$, we say the scattering length is infinite.

The scattering length a is a natural scattering parameter because, by (112), $\lim_{E\to 0} f_{\ell=0}(E) = a$. Moreover, it can be shown under many circumstances that $\sum_{\ell\geq 1} k^{-2} \sin^2 \delta_\ell(k^2) \to 0$ as $k \to 0$ so that $\lim_{E\to 0} \sigma_{\text{tot}}(E) = 4\pi a^2$ by (111).

E. Jost functions and Levinson's theorem

Theorem XI.53 relates the phase shift to solutions of the radial Schrödinger equation, at least when V is regular. To discuss general V, and also in order to discuss systematically the solutions of (114), it is useful to rewrite the Schrödinger equation with boundary conditions as an integral equation. As a dividend of our development of the integral equation approach, we shall relate the number of spherically symmetric eigenfunctions to the s-wave phase shift. We discuss only the $\ell = 0$ case. References for the general case can be found in the Notes.

Definition **The Schrödinger integral equation with regular boundary conditions at 0**, or, for short the **regular equation** is

$$f(x) = x + \int_0^x (x - y)[V(y) - k^2]f(y)\, dy \tag{125}$$

Definition Let $k \neq 0$. The **Schrödinger integral equation with Jost boundary conditions at** ∞, or, for short the **Jost equation** is

$$f(x) = e^{-ikx} - \int_x^\infty \frac{\sin k(x-y)}{k} V(y) f(y)\, dy \tag{126}$$

When V is sufficiently regular, for example if V is continuous, (125) and (126) are equivalent to the Schrödinger differential equation (114) with appropriate boundary conditions. There is a systematic method known as the method of variation of parameters which can be used to rewrite second-order differential equations with boundary conditions as integral equations (see Appendix 2).

Theorem XI.56 Suppose that V is a measurable function obeying $N(x) \equiv \int_0^x y|V(y)|\, dy < \infty$ for each $x > 0$. Then, for each $k \in \mathbb{C}$, the regular equation (125) has a unique solution $\varphi(x, k)$ that is locally bounded on $(0, \infty)$ and obeys $\overline{\lim}_{x\to 0} |x^{-1}\varphi(x)| < \infty$. Moreover, $\varphi(x, k)$ is continuously differentiable in x on $[0, \infty)$ with $\varphi(0, k) = 0$, $\varphi'(0, k) = 1$ and, for each fixed x, $\varphi(x, k)$ and $\varphi'(x, k)$ are entire functions of k obeying

$$|\varphi(x, k)| \leq x \exp[N(x) + \tfrac{1}{2}|k|^2 x^2]$$
$$|\varphi'(x, k)| \leq \exp[N(x) + \tfrac{1}{2}|k|^2 x^2]$$

In addition $\overline{\varphi(x, k)} = \varphi(x, \bar{k})$. φ is called the **regular solution.**

Proof Let $\psi(x) = f(x)/x$ so that to solve (125), we seek ψ obeying

$$\psi(x) = 1 + \int_0^x K(x, y)\psi(y)\, dy \tag{127}$$

where

$$K(x, y) = y\left(1 - \frac{y}{x}\right)(V(y) - k^2)$$

By iterating (127), we obtain a formal series

$$\psi(x) = \sum_{n=0}^\infty \psi_n(x) \tag{128}$$

where

$$\psi_0(x) = 1, \qquad \psi_n(x) = \int_0^x K(x, y)\psi_{n-1}(y)\, dy$$

We shall prove inductively that

$$|\psi_n(x)| \le (n!)^{-1}P(x)^n \tag{129}$$

where

$$P(x) = N(x) + \tfrac{1}{2}|k|^2x^2$$

(129) certainly holds if $n = 0$. If $0 \le y \le x$, then

$$|K(x, y)| \le y(|V(y)| + |k^2|)$$

so if ψ_n obeys (129), then

$$\begin{aligned}|\psi_{n+1}(x)| &\le \int_0^x y(|V(y)| + |k|^2)(n!)^{-1}P(y)^n\,dy\\ &= (n!)^{-1}\int_0^x (P(y))^n\,\frac{dP}{dy}\,dy\\ &= [(n+1)!]^{-1}(P(x))^{n+1}\end{aligned}$$

so (129) holds by induction.

We conclude that (128) converges uniformly on compacts in x and k. Since each $\psi_n(x)$ is analytic in k (it is a polynomial!), the limiting function is analytic in k. ψ obeys (127), so φ obey (125). The bound on φ follows from (129). The analyticity of φ' in k and the bound on φ' follow from the formula

$$\varphi'(x, k) = 1 - \int_0^x y(V(y) - k^2)\psi(y, k)\,dy$$

and the bound (129). Uniqueness is left to the reader (Problem 84). ▌

Theorem XI.57 Suppose that V is a measurable function obeying $\int_x^\infty |V(y)|\,dy < \infty$ for each $x > 0$. Define $Q_k(x)$ by

$$Q_k(x) = \int_x^\infty (1 + |k|y)^{-1}4y|V(y)|e^{(\operatorname{Im} k + |\operatorname{Im} k|)y}\,dy$$

Then:

(a) For each $k \in \mathbb{C}$, with $\operatorname{Im} k \le 0$, and $k \ne 0$, the Jost equation (126) has a unique solution $\eta(x, k)$ obeying $\lim_{x\to\infty} |e^{ikx}\eta(x, k)| < \infty$. Moreover, $\eta(x, k)$ is continuously differentiable in x on $[0, \infty)$ with $\lim_{x\to\infty} e^{ikx}\eta(x, k) = 1$ and $\lim_{x\to\infty} e^{ikx}\eta'(x, k) = -ik$. For each fixed x,

$\eta(x, k)$ and $\eta'(x, k)$ are functions analytic in $\{k \mid \operatorname{Im} k < 0\}$, continuous in $\{k \mid \operatorname{Im} k \le 0;\ k \ne 0\}$, obeying

$$|\eta(x, k) - e^{-ikx}| \le e^{(\operatorname{Im} k)x} |e^{Q_k(x)} - 1| \tag{130a}$$

$$|\eta'(x, k) + ike^{-ikx}| \le e^{(\operatorname{Im} k)x} e^{Q_k(x)} \int_x^\infty |V(y)|\, dy \tag{130b}$$

(b) If, in addition, $\int_0^\infty x|V(x)|\, dx < \infty$, then $\eta(x, k)$ may be extended to $k = 0$ in such a way that $\eta(x, k)$ is continuous on $\{k \mid \operatorname{Im} k \le 0\}$. Moreover, (130) continues to hold.

(c) If, in addition, $\int_x^\infty e^{my}|V(y)|\, dy < \infty$, then $\eta(x, k)$ can be extended, for each x, to a function analytic in $\{k \mid \operatorname{Im} k < \frac{1}{2}m\}$. Moreover, (130) continues to hold.

In each case, η obeys $\overline{\eta(x, k)} = \eta(x, -\bar{k})$. η is called the **Jost solution.**

Proof The idea is very similar to the proof of Theorem XI.56, so we only sketch the proof leaving the details to the reader (Problem 85). (126) is formally solved by the series

$$\eta(x, k) = \sum_{n=0}^{\infty} \eta_n(x, k)$$

where $\eta_0(x, k) = e^{-ikx}$ and

$$\eta_n(x, k) = \int_x^\infty k^{-1}[\sin k(y - x)]V(y)\eta_{n-1}(y, k)\, dy$$

From the bound

$$\frac{|\sin k(x - y)|}{|k|} \le \frac{4y}{1 + |k|y} \exp[|\operatorname{Im} k|y + (\operatorname{Im} k)x], \qquad y \ge x \ge 0$$

one obtains by induction

$$|\eta_n(x, k)| \le (n!)^{-1} Q_k(x)^n$$

If we interpret $k^{-1} \sin k(x - y)$ as $(x - y)$ when $k = 0$, then these bounds continue to hold when $k = 0$. Each $\eta_n(x, k)$ is easily seen to be analytic in the interior of the region where $Q_k(1) < \infty$ and continuous on the boundary. The assertions of the theorem are proven by summing the series. ∎

We now define the Jost function, which we shall see is intimately connected to the scattering amplitude.

Theorem XI.58 Let V obey

$$\int_0^x |y|\,|V(y)|\,dy + \int_x^\infty |V(y)|\,dy < \infty$$

for each x. Then:

(a) $\eta(k) \equiv \eta(x, k)\varphi'(x, k) - \eta'(x, k)\varphi(x, k)$ is independent of x. $\eta(k)$ is called the **Jost function**.
(b) $\eta(k)$ is analytic in $\{k \mid \operatorname{Im} k < 0\}$ and continuous in $\{k \mid \operatorname{Im} k \le 0;\ k \ne 0\}$. If V obeys $\int_1^\infty e^{my}|V(y)|\,dy < \infty$, for some $m > 0$, then $\eta(k)$ is analytic in $\{k \mid \operatorname{Im} k < \frac{1}{2}m\}$.
(c) If k is real and nonzero, then $\eta(k) \ne 0$, $\eta(-k) = \overline{\eta(k)}$ and

$$\frac{\eta(k)}{\eta(-k)} = e^{2i\delta_0(k)}$$

where $\delta_0(k)$ is the s-wave phase shift.
(d) All the zeros of $\eta(k)$ in $\{k \mid \operatorname{Im} k < 0\}$ are simple. They lie on the imaginary axis and k is a zero if and only if k^2 is an $\ell = 0$ bound state energy.
(e) $\displaystyle\lim_{\substack{k\to\infty \\ \operatorname{Im} k \le 0}} \eta(k) = 1.$

Proof (a) First suppose that $V \in C_0^\infty(0, \infty)$. Then η and φ both obey the differential equation $-u'' + Vu = k^2 u$ so $\eta\varphi' - \eta'\varphi$ is constant since it is the Wronskian of two solutions (an explicit computation shows that $(\eta\varphi' - \eta'\varphi)' = 0$). If V is an arbitrary potential obeying the hypothesis, we can find $V_n \in C_0^\infty$, so that $\int_0^1 y|V_n - V|\,dy + \int_1^\infty |V_n - V|\,dy \to 0$ as $n \to \infty$. By the construction of φ and η, we conclude that $\varphi_n \to \varphi$, $\varphi_n' \to \varphi'$, $\eta_n \to \eta$, $\eta_n' \to \eta'$ pointwise, so (a) holds in general. For the proof of our assertion that η is called the Jost function, see the Notes.

(b) This follows from the analyticity properties of φ, φ', η, η' stated in Theorems XI.56 and XI.57.

(c) Since $\overline{\varphi(x, k)} = \varphi(x, k) = \varphi(x, -k)$ and $\overline{\eta(x, k)} = \eta(x, -k)$ when k is real, we conclude that $\eta(-k) = \overline{\eta(k)}$. Next we claim that

$$\varphi(x, k) = (2ik)^{-1}\{\eta(k)\eta(x, -k) - \eta(-k)\eta(x, k)\} \tag{131}$$

We shall prove (131) and the basic relation $\eta(k)/\eta(-k) = e^{2i\delta_0}$ for $V \in C_0^\infty(0, \infty)$. The general case then follows by a limiting argument as in the proof of (a). Suppose that $\operatorname{supp} V \subset [a, b]$, $0 < a < b < \infty$. Then $\varphi(\cdot, k)$, $\eta(\cdot, k)$, and $\eta(\cdot, -k)$ are all solutions of $-u'' + Vu = k^2 u$. Moreover, for $x > b$, $\eta_\pm(x) \equiv \eta(x, \pm k) = e^{\pm ikx}$, so $\eta_\pm$ are linearly independent and their

Wronskian $W(\eta_+, \eta_-) = \eta_+ \eta'_- - \eta_- \eta'_+$ is $2ik$. Thus

$$\varphi = W(\eta_+, \eta_-)^{-1}[W(\eta_+, \varphi)\eta_- - W(\eta_-, \varphi)\eta_+]$$

which is (131).

(131), $\eta(k) = \overline{\eta(-k)}$, and the fact that φ is not identically zero imply that $\eta(k) \neq 0$. Moreover, since $\eta_\pm(x) = e^{\pm ikx}$ for $x > b$, we see that

$$\varphi(x) = k^{-1}|\eta(k)| \sin(kx + d(k))$$

for $x > b$ if $\eta(k) = |\eta(k)|e^{id(k)}$. By Theorem XI.53, we conclude that $d(k) = \delta_0(k)$ (mod 2π).

(d) We first claim that $(-\Delta + V - k^2)(x^{-1}\varphi(x, k)) = 0$ where $-\Delta$ is to be interpreted in distributional sense. For this holds if $V \in C_0^\infty(0, \infty)$ and so for general V by a limiting argument. If $\eta(k) = 0$, then φ is a constant multiple of η and so in L^2 at infinity. Thus k is purely imaginary and k^2 is an eigenvalue.

Conversely, suppose that $V \in C_0^\infty$ and that k^2 is an $\ell = 0$ eigenvalue of $-\Delta + V$. Since V falls off exponentially, η is an entire function, so (131) holds for all k. Then, by this analytic continuation of (131), $\eta(k) = 0$. By a limiting argument, this extends to all V.

Finally, we must show that the zeros of η are simple. We first note that if $u = x^{-1}\varphi$ and $v = x^{-1}\,\partial\varphi/\partial k$, then

$$(-\Delta + V - k^2)u = 0 \tag{132a}$$

$$(-\Delta + V - k^2)v = 2ku \tag{132b}$$

in distributional sense. Moreover, if $\eta(k_0) = (\partial\eta/\partial k)(k_0) = 0$, then one can show that

$$\frac{\partial\varphi}{\partial k} = c_1\eta + c_2\,\frac{\partial\eta}{\partial k}$$

so $v \in L^2$. But if $u, v \in L^2$, then (132) is inconsistent with $u \neq 0$ since

$$2k\|u\|^2 = (u, (-\Delta + V - k^2)v) = 0$$

Thus, if $\eta(k_0) = 0$, then $\partial\eta/\partial k \neq 0$ at k_0, so the zeros of η are simple.

(e) By (130a) and $\eta(k) = \eta(0, k)$,

$$|\eta(k) - 1| \leq |\exp Q_k(0) - 1|$$

if $\operatorname{Im} k \leq 0$. Thus it suffices to prove that

$$\lim_{k\to\infty} \int_0^\infty \frac{y|V(y)|}{1 + |k|y} = 0$$

and this follows from the monotone convergence theorem. ∎

One of the more spectacular consequences of the machinery of Jost functions is:

Theorem XI.59 (Levinson's theorem) Let V obey $\int_0^\infty x\,|V(x)|\,dx < \infty$ and let η be the Jost function and δ_0 the s-wave phase shift normalized by $\lim_{k\to\infty} \delta_0(k^2) = 0$. Then

$$\delta_0(0) = \begin{cases} n_0\pi, & \text{if} \quad \eta(0) \neq 0 \\ (n_0 + \frac{1}{2})\pi, & \text{if} \quad \eta(0) = 0 \end{cases}$$

where n_0 is the number of eigenvalues with spherically symmetric eigenfunctions for $-\Delta + V$.

Proof We consider the case $\eta(0) \neq 0$. The case $\eta(0) = 0$ is left to the problems. By (131), all $\ell = 0$ eigenfunctions have $k^2 < 0$, so by Theorem XI.58d, n_0 is the number of zeros of $\eta(k)$ in the lower half-plane. Let $0 < \theta < \frac{1}{2}\pi$. Pick R_0, so that $|\eta(k) - 1| < 2\sin(\frac{1}{2}\theta)$ for $|k| \geq R_0$, $\operatorname{Im} k \leq 0$. By Theorem XI.58e, such an R_0 exists. Consider the integral of η'/η around the contour $C = C_1 \cup C_2$ in Figure XI.10. The poles of η'/η are at the zeros of η and since these zeros are simple, the residues are equal to 1. Thus

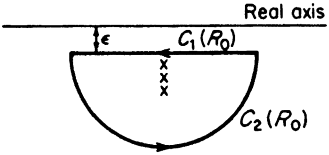


FIGURE XI.10 A contour for Levinson's theorem.

$$n_0 = (2\pi i)^{-1} \int_C \frac{\eta'}{\eta}\, dz$$

Now $i^{-1}\eta'/\eta = d(\arg \eta)/dz$, so in the limit as $\varepsilon \to 0$, the contribution of C_1 is $\pi^{-1}(\delta_0(0) - \delta_0(R_0^2))$. Since $|\arg \eta| < \theta$ on all of $C_2(R_0)$ by the choice of R_0, we conclude that

$$|\pi^{-1}[\delta_0(0) - \delta_0(R_0^2)] - n_0| \leq 2\theta$$

Taking $R_0 \to \infty$, $\theta \to 0$, we see that $\delta_0(0) = n_0\pi$. ∎

We saw in Section 7 that the poles in the upper half-plane of the forward scattering amplitude can occur only at points k where k^2 is an eigenvalue of $-\Delta + V$. The formula

$$f_{\ell=0}(k^2) = 2ik^{-1}(\eta(k) - \eta(-k))/\eta(-k)$$

which follows from Theorem XI.58c together with the fact that the only zeros of $\eta(-k)$ are at points where k^2 is an eigenvalue, suggests that the poles of $f_{\ell=0}(k^2)$ in the upper half-plane are also connected only to bound states. This is false. In the first place, for general potentials the analyticity domains of $\eta(k)$ and $\eta(-k)$ are disjoint and there may be no continuation for $f_{\ell=0}$. Moreover, it can happen that $\eta(k)$ has a meromorphic continuation to the upper half-plane with poles at certain points. These poles will produce poles in $f_{\ell=0}$ which do not correspond to bound states. This phenomenon will be discussed further in the next subsection.

F. Analyticity of the partial wave amplitude for generalized Yukawa potentials

In Section 7 we saw that the full scattering amplitude $f(E, \cos\theta)$ has analyticity properties in E at $\cos\theta = 1$ under rather general circumstances. Analyticity at $\theta \neq 0$ required some exponential falloff. Not surprisingly then, analyticity properties for $f_0(k)$, the s-wave scattering amplitude, requires exponential falloff. From the results of part E, and the formula $ss_0(k^2) = \eta(k)/\eta(-k)$ and $f_0(k^2) = (2ik)^{-1}[s_0(k^2) - 1]$, we see that:

Theorem XI.60 If $\int_1^\infty e^{my}|V(y)|\,dy + \int_0^1 y|V(y)|\,dy < \infty$, then the s-wave partial wave amplitude is real analytic on $(0, \infty)$ and has a meromorphic continuation from the upper edge of the real axis into the parabolic region, $\{E \mid |E| - \operatorname{Re} E \leq \frac{1}{2}m^2,\ E \text{ not a positive real}\}$ (see Figure XI.11), with poles precisely at the energies of bound states in the region $E > -\frac{1}{4}m^2$.

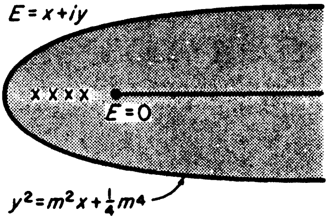


FIGURE XI.11 Analyticity region for $f_0(E)$, general case.

Proof Let $G(k) = \eta(k)/\eta(-k)$. Then G is analytic in the region $|\operatorname{Im} k| \leq \frac{1}{2}m$. In the region $\operatorname{Im} k > 0$, $G(k)$ can have poles only when $\eta(-k) = 0$. If $\eta(-k) = 0$, $\eta(k) \neq 0$ by the analytic continuation of (131). Thus G has poles precisely at zeros of $\eta(-k)$. The theorem now follows from the formula $f_0(E) = (2i\sqrt{E})^{-1}[G(\sqrt{E}) - 1]$. ▌

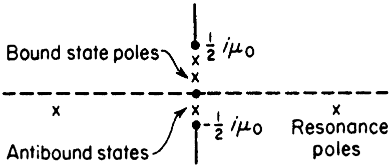
For the generalized Yukawa potentials defined in Section 7, we can say much more (μ_0 is the constant occurring in the definition of generalized Yukawa potentials):

Theorem XI.61 Let $f_0(E)$ be the *s*-wave scattering amplitude for a generalized Yukawa potential. Then there is a function $F(E)$, meromorphic in $D = \mathbb{C}\backslash([0, \infty) \cup (-\infty, -(\frac{1}{2}\mu_0)^2])$, so that for $E \in (0, \infty)$

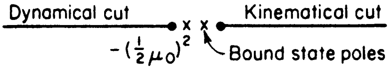
$$f_0(E) = \lim_{\varepsilon \downarrow 0} F(E + i\varepsilon)$$

The only poles of F *in* D occur on the negative axis at bound state energies, and there is a pole at each such energy in $(-(\frac{1}{2}\mu_0)^2, 0)$. Moreover, $f_0(E)$ is real analytic on $(0, \infty)$.

Before turning to the proof of Theorem XI.61, we make a series of remarks, one of which explains the reason for emphasizing that it is only the poles *in D* that are described in the theorem. First, one can prove that f is analytic in $\mathbb{C}\backslash([0, \infty) \cup (-\infty, -\mu_0^2])$. Secondly, we shall actually prove more than is stated in the theorem. We shall show that the function $G(k)$ defined by $G(k) = F(k^2)$ for $\text{Im } k > 0$ has a meromorphic continuation to $\mathbb{C}\backslash([\frac{1}{2}i\mu_0, i\infty) \cup (-i\infty, -\frac{1}{2}i\mu_0])$—see Figure XI.12. As a result, the cut from 0 to ∞ in $F(E)$ is due entirely to the use of the variable $E = k^2$, and one can continue onto a second sheet by continuing past this cut. Poles of $F_0(E)$ on the second sheet with $\text{Im } E \neq 0$ (equivalently, poles of $G(k)$ at points with $\text{Re } k \neq 0$, $\text{Im } k < 0$) are called **resonance poles**—one can show that they correspond precisely to the resonances that will be discussed in Section XII.6 since the generalized Yukawa potentials are dilation analytic. Poles corresponding to $k \in (-\frac{1}{2}i\mu_0, 0)$ are called **antibound states**.



(a) Analyticity region for $G(-k)$



(b) Analyticity region for $F(E)$

FIGURE XI.12 (a) Region for $G(-k)$, (b) analyticity region for $F(E)$.

Since the cut in $[0, \infty)$ is due entirely to the use of the variable E instead of k, it is often called the **kinematical cut**. It is also called the **unitarity cut** since its discontinuity is given by the unitarity relation

$$F(E + i0) - F(E - i0) = 2 \operatorname{Im} f_0(E) = E^{1/2} |f_0(E)|^2$$

The cut in $(-\infty, -(\frac{1}{2}\mu_0)^2]$ is directly related to the potential in that its discontinuities can be computed directly from the potential by an iterative scheme (see the Notes). This cut is called the **dynamical cut**. The phrase **left-hand cut** and **right-hand cut** are sometimes used in place of dynamical cut and kinematical cut.

Finally, there is one subtle point. It can happen that the left-hand cut partly "degenerates into poles," that is, that $F(E)$ has a meromorphic continuation into a region including $(-a, -(\frac{1}{2}\mu_0)^2)$, $a > (\frac{1}{2}\mu_0)^2$, with poles in this region. The poles of $F(E)$ in this interval may not be connected with bound states; for this reason, they are often called **false poles**. In fact, there exist distinct generalized Yukawa potentials, V_1 and V_2, for which the corresponding s-wave partial wave amplitudes are equal but which are distinguished by the fact that all the poles of $F(E)$ are associated with bound states of $-\Delta + V_1$ while the leftmost pole of $F(E)$ is not associated with a bound state of $-\Delta + V_2$ but rather with its dynamical cut! This example is especially surprising because of Levinson's theorem which tells us that $F(E + i0)$ determines the number of bound states and so, one would assume, the number of bound state poles. The point is that if a bound state energy is not in $(-a, -(\frac{1}{2}\mu_0)^2)$, the pole which one would expect to be there can have a zero residue. Thus, while $-\Delta + V_1$ and $-\Delta + V_2$ have the same number of bound states of angular momentum zero, they have different numbers of "bound state poles."

Throughout the proof of Theorem XI.61, we shall suppose that V is of the form $V(x) = x^{-1}e^{-\mu_0 x}$. It is a simple exercise to extend the proof to generalized Yukawa potentials. The main idea is to use the analyticity of $V(x)$ in the region $\{x \mid \operatorname{Re} x > 0\}$ to extend the Jost function $\eta(k)$ in k. There is thus a close connection between these ideas and the dilation analytic ideas of Sections XII.6 and XIII.10. Our extension of $\eta(k)$ is in two steps:

Lemma 1 The function $\eta(x, k)$ which is defined initially on $\{\langle x, k\rangle \mid x \in (0, \infty), \operatorname{Im} k \leq 0\}$ can be extended to $\Omega = \{\langle x, k\rangle \mid \operatorname{Re} x > 0, \operatorname{Im} k \leq 0\}$ in such a way as to be a jointly analytic function of x and k in Ω^{int}, continuous in Ω. Moreover, in Ω, it obeys the differential equation

$$-\frac{d^2}{dx^2}\eta(x, k) + V(x)\eta(x, k) = k^2\eta(x, k)$$

and in the region $\Omega' = \{\langle x, k\rangle \in \Omega \mid |x| > 1\}$, it obeys the bound

$$|\eta(x, k) - e^{-ikx}| \le e^{\text{Im}(kx)}\{\exp[\mu_0^{-1}|k|^{-1}e^{-\mu_0 \text{ Re } x}] - 1\} \tag{133}$$

Proof We shall show that η can be extended to Ω' obeying (133). By the same method, one can extend η to the region $\{\langle x, k\rangle \in \Omega \mid |x| > \varepsilon\}$ and so to all of Ω. Since the differential equation is valid when x is real, it holds for all x by analytic continuation. Fix k with $\text{Im } k \le 0$. Define $\eta_n(x, k)$ inductively on Ω' by

$$\eta_0(x, k) = e^{-ikx}$$

$$\eta_n(x, k) = \int_0^\infty k^{-1} (\sin ky)V(y + x)\eta_{n-1}(y + x, k)\, dy$$

A change of variables shows that when x is real, $\eta_n(x, k)$ agrees with the function defined in the proof of Theorem XI.57. Moreover, we claim the following bound holds in Ω':

$$|\eta_n(x, k)| \le (n!)^{-1}e^{\text{Im}(kx)}(\mu_0|k|)^{-n}e^{-n\mu_0 \text{Re } x} \tag{134}$$

(134) certainly holds when $n = 0$; and if it holds for some n, then

$$\begin{aligned} |\eta_{n+1}(x, k)| &\le (n!)^{-1}(\mu_0\,|k|)^{-n} \\ &\qquad \times \int_0^\infty |k|^{-1}e^{y|\text{Im } k|}e^{-\mu_0(\text{Re } x + y)(n+1)}e^{\text{Im}(kx) + (\text{Im } k)y}\, dy \\ &= [(n + 1)!]^{-1}(\mu_0|k|)^{-n-1}e^{-(n+1)\mu_0 \text{ Re } x} \end{aligned}$$

since $|\text{Im } k| + \text{Im } k = 0$ when $\text{Im } k \le 0$ and $(x + y)^{-1} \le 1$ when $|x| > 1$, $\text{Re } x > 0$, $y \in (0, \infty)$. This proves (134) inductively.

By (134), the integral defining η_n converges absolutely, so η_n is analytic in $(\Omega')^{\text{int}}$. Since $\sum_n \eta_n$ converges absolutely by (134), the limit has the required analyticity and obeys the bound (133). ▌

Lemma 2 The Jost function $\eta(k)$ can be analytically continued to $\mathbb{C}\backslash[\frac{1}{2}i\mu_0, i\infty)$.

Proof Since we already know by Theorem XI.58 that $\eta(k)$ is analytic in $\{k \mid \text{Im } k \le \frac{1}{2}\mu_0\}$, we need only prove that $\eta(k)$ has an analytic continuation to every half-plane of the form $\{k \mid \text{Im}(e^{-i\alpha}k) \le 0\}$ for each $\alpha \in (-\frac{1}{2}\pi, \frac{1}{2}\pi)$. Fix such an α and define $\tilde{\eta}$ on $\{\langle y, k\rangle \mid y \in \mathbb{R}, \text{Im } k \le 0\}$ by

$$\tilde{\eta}(y, k) = \eta(e^{-i\alpha}y, k)$$

where $\eta(x, k)$ is continued to complex x by using Lemma 1. Then $\tilde{\eta}$ obeys the differential equation

$$\left(-\frac{d^2}{dy^2} + \tilde{V}(y)\right)\tilde{\eta}(y, k) = \tilde{k}^2\tilde{\eta}(y, k) \tag{135}$$

where $\tilde{V}(y) = e^{-2i\alpha}V(e^{-i\alpha}y)$ and $\tilde{k} = e^{-i\alpha}k$. Moreover, by (133),

$$|\tilde{\eta}(y, k) - e^{-i\tilde{k}y}| \to 0 \tag{136}$$

as $y \to \infty$, so long as $\text{Im}\ \tilde{k} \le 0$, $\text{Im}\ k \le 0$. In the proof of Theorem XI.57, the reality of V was not used anywhere, so we know that (135) has a unique solution $\eta_1(y, \tilde{k})$ for $\{\langle y, k\rangle \mid y \in [0, \infty),\ \text{Im}\ \tilde{k} \le 0\}$ obeying (136). Thus $\tilde{\eta}(y, k)$ and $\eta_1(y, e^{-i\alpha}k)$ agree in the region $\{k \mid \text{Im}\ k \le 0, \text{Im}(e^{-i\alpha}k) \le 0\}$ so η_1 is an analytic continuation of $\tilde{\eta}$ to $\{k \mid \text{Im}(e^{-i\alpha}k) \le 0\}$. In particular, $\eta(k) = \tilde{\eta}(0, k)$ has a continuation to $\{k \mid \text{Im}(ke^{-i\alpha}) \le 0\}$. ▮

Proof of Theorem XI.61 Since $f_0(k^2) = (2ik)^{-1}[e^{2i\delta_0(k)} - 1]$, we need only prove the analyticity statements for $s_0(k) = e^{2i\delta_0(k)}$. But since $s_0(k) = \eta(k)/\eta(-k)$, we see that $s_0(k)$ is meromorphic in $D = \{k \mid k \notin [\frac{1}{2}i\mu_0, \infty) \cup (-\infty, -\frac{1}{2}i\mu_0]\}$ and the only poles in $D \cap \{k \mid \text{Im}\ k > 0\}$ occur at points k_0 with $\eta(-k_0) = 0$. Moreover, as in the proof of Theorem XI.60, poles occur at all such k_0. ▮

G. The Kohn variational principle

In the discussion of the variable phase method, we saw that the scattering length, a, was an important parameter since, under some circumstances, $\lim_{E\to 0} \sigma_{\text{tot}}(E) = 4\pi a^2$. Recall that the scattering length for potentials V with compact support was determined by finding a suitable normalized solution of $-\varphi'' + V\varphi = 0$, $\varphi(0) = 0$, with $\varphi(r) = r + a$ for r large. Consider real-valued functions, ψ, on $[0, \infty)$ of the form

$$\psi = \alpha r + \beta + g \tag{136a}$$

with g smooth, g, g', g'' falling off faster than any polynomial and $\psi(0) = 0$. Let Q be the set of such functions and let $\alpha(\psi)$, $\beta(\psi)$ be the constants in (136a).

For ψ, η in Q, we can define a natural object,

$$(\psi, h\eta) = \int_0^\infty \psi(r)(-\eta''(r) + V(r)\eta(r))\, dr$$

since $\bar{\psi}(-\eta'')$ is in L^1. However, it is false that $(\psi, h\eta)$ and $(\eta, h\psi)$ are equal; rather

$$(\psi, h\eta) - (\psi, h\eta) = \int_0^\infty (\psi''\eta - \psi\eta'')\, dr$$

$$= \alpha(\psi)\beta(\eta) - \beta(\psi)\alpha(\eta) \tag{136b}$$

since the boundary term at infinity does not vanish. Take $\eta = \varphi$, the solution of $h\varphi = 0$ and suppose that ψ is such that $\alpha(\psi) = 1$. Then $(\psi, h\eta) = 0$ so we have that

$$\begin{aligned} a &= \beta(\psi) - (h\psi, \varphi) \\ &= \beta(\psi) - (h\psi, \psi) + (h\psi, (\psi - \varphi)) \\ &= \beta(\psi) - (h\psi, \psi) + (h(\psi - \varphi), (\psi - \varphi)) \end{aligned}$$

The equation

$$a = \beta(\psi) - (h\psi, \psi) + (h(\psi - \varphi), (\psi - \varphi)) \tag{136c}$$

is called the **Kohn variational principle**. Under some circumstances, it can be used to get a rigorous bound on the scattering length:

Theorem XI.61.5 (Rosenberg–Spruch bound) Suppose that $V \in C_0^\infty$ is central and that $-\Delta + V$ has no negative eigenvalues. Let ψ be any function in Q with $\alpha(\psi) = 1$. Then the scattering length a obeys

$$a \geq \beta(\psi) - (h\psi, \psi) \tag{136d}$$

Proof By the Kohn principle, (136c), it suffices that we show $(h\eta, \eta) \geq 0$ for $\eta \in Q$ with $\alpha(\eta) = 0$. Let g be C^∞ on $[0, \infty)$ with $g = 1$ (respectively, $g = 0$) for $r < 1$ (respectively, $r > 2$) and let $g_R(x) = g(x/R)$. Then ηg_R is in L^2 so $0 \leq (g_R \eta, h(g_R \eta))$ by the hypothesis that there are no negative eigenvalues. But $(g_R \eta, h(g_R \eta)) = X + Y + Z$ where

$$\begin{aligned} X &= (g_R^2 \eta, h\eta) \to (\eta, h\eta) && \text{as} \quad R \to \infty \\ Y &= -(g_R \eta, \eta g_R'') \to 0 && \text{as} \quad R \to \infty \\ Z &= -2(g_R \eta, (\nabla\eta)\nabla g_R) \to 0 && \text{as} \quad R \to \infty \end{aligned}$$

where the convergence results follow from $h\eta \leq d_1(1 + r)^{-2}$, $\eta \leq d_2$, $\nabla\eta \leq d_3(1 + r)^{-2}$, $\|g_R''\|_\infty \leq d_4 R^{-2}$, and $\|g_R'\|_\infty \leq d_5 R^{-1}$. Thus $(\eta, h\eta) \geq 0$. ∎

Note that whether (136d) yields an upper or a lower bound on a^2 depends on whether we know that a is positive or negative. For example, by Corollary 3 to Theorem XI.54 and Theorem XI.55, we see that if V is everywhere positive, then (136d) provides an upper bound on a^2.

Appendix 1 to XI.8: Legendre polynomials and spherical Bessel functions

Scattering theory requires some information about certain classes of special functions. The basic properties of Legendre polynomials are most easily derived by defining them in terms of a generating function:

Definition For each $z \in \mathbb{C}$, the function

$$F(x, z) = (1 - 2zx + x^2)^{-1/2}$$

is analytic near $x = 0$. The **Legendre polynomials** $P_\ell(z)$ are defined by

$$P_\ell(z) = (\ell!)^{-1}\left(\frac{d}{dx}\right)^\ell F(x, z)\bigg|_{x=0}$$

or equivalently by

$$(1 - 2xz + x^2)^{-1/2} = \sum_{\ell=0}^{\infty} P_\ell(z)x^\ell$$

Theorem XI.62

(a) $P_\ell(z)$ is a polynomial of degree ℓ with real coefficients.

(b) $P_\ell(1) = 1$; $P_\ell(-z) = (-1)^\ell P_\ell(z)$.

(c) Define f on $\mathbb{R}^3$ by $f(\mathbf{x}) = r^\ell P_\ell(\cos\theta)$ where $r = |\mathbf{x}|$ and $\cos\theta = x_3/r$. Then $-\Delta f = 0$.

(d) (Legendre's equation)

$$(1 - z^2)\frac{d^2}{dz^2}P_\ell(z) - 2z\frac{d}{dz}P_\ell(z) + \ell(\ell + 1)P_\ell(z) = 0$$

(e) $\displaystyle\int_{-1}^{1} P_\ell(z)P_m(z)\,dz = \frac{2}{2\ell + 1}\,\delta_{\ell m}$.

(f) $\{(\ell + \frac{1}{2})^{1/2}P_\ell(z)\}_{\ell=0}^{\infty}$ are an orthonormal basis for $L^2((-1, 1), dz)$.

Proof (a) By the binomial theorem,

$$(1 - 2xz + x^2)^{-1/2} = \sum_{m=0}^{\infty} \binom{-\frac{1}{2}}{m} (-2xz + x^2)^m$$

for x small, where $\binom{k}{m} = k(k-1) \cdots (k-m+1)/m!$ For fixed ℓ, only the terms with $m \le \ell$ can contribute to $(d/dx)^\ell f(x, z)|_{x=0}$. By using the binomial theorem on $(-2xz + x^2)^m$, we see that $\sum_{m=0}^{\ell} \binom{-\frac{1}{2}}{m}(-2xz + x^2)^m$ is a polynomial of two variables of degree ℓ in z. Furthermore, $P_\ell(z) = (-2z)^\ell \binom{-\frac{1}{2}}{\ell} + O(z^{\ell-2})$ so that P_ℓ has degree precisely ℓ.

(b) Since $(1 - 2x + x^2)^{-1/2} = (1-x)^{-1} = \sum_{n=0}^{\infty} x^n$, we see that $P_\ell(1) = 1$. From $f(-x, -z) = f(x, z)$ we obtain $P_\ell(-z) = (-1)^\ell P_\ell(z)$.

(c) Fix $R > 0$. In the region $\{\langle \mathbf{r}, \mathbf{r}' \rangle \in \mathbb{R}^6 \,|\, r < R < r'\}$ define $g(\mathbf{r}, \mathbf{r}') = |\mathbf{r} - \mathbf{r}'|^{-1}$. Then, for fixed r', $-\Delta g = 0$ in the region $\{\mathbf{r} \,|\, r < R\}$. Let $\mathbf{r}' = \langle 0, 0, \alpha \rangle$ and $x = r/\alpha$. Then

$$\begin{aligned} |\mathbf{r} - \mathbf{r}'|^{-1} &= (r^2 + r'^2 - 2rr' \cos\theta)^{-1/2} \\ &= (r')^{-1}(1 + x^2 - 2x\cos\theta)^{-1/2} \\ &= (r')^{-1} \sum_{\ell=0}^{\infty} P_\ell(\cos\theta) x^\ell = \sum_{\ell=0}^{\infty} (r')^{-\ell-1} r^\ell P_\ell(\cos\theta) \end{aligned}$$

where we have used the fact that for $z \in (-1, 1)$, $f(x, z)$ has radius of convergence 1 in x. Thus $r^\ell P_\ell(\cos\theta)$ is given inductively by

$$r^\ell P_\ell(\cos\theta) = \lim_{r' \to \infty} (r')^{\ell+1} \left[g(\mathbf{r}, \mathbf{r}') - (r')^{-1} \sum_{k=0}^{\ell-1} P_k(\cos\theta) \left(\frac{r}{r'}\right)^k \right]$$

where the convergence is uniform in $\{\mathbf{r} \,|\, r < R\}$. By induction in ℓ using the fact that a uniform limit of harmonic functions is harmonic (Problem 89), we conclude that $r^\ell P_\ell(\cos\theta)$ is harmonic.

(d) Since

$$\Delta = r^{-2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + (r^2 \sin\theta)^{-1} \frac{\partial}{\partial\theta} (\sin\theta) \frac{\partial}{\partial\theta} + (r^2 \sin^2\theta)^{-1} \frac{\partial^2}{\partial\varphi^2}$$

(d) follows from (c).

(e) Legendre's equation may be written

$$\frac{d}{dz}(1 - z^2) \frac{d}{dz} P_\ell(z) = -\ell(\ell+1) P_\ell(z)$$

Thus, if $\ell \ne m$, $\int_{-1}^{1} P_\ell(z) P_m(z)\, dz = 0$ since $(d/dz)(1 - z^2)(d/dz)$ is symmetric.

Now, for small x, we compute that on the one hand

$$\int_{-1}^{1}\left(\sum_{\ell=0}^{\infty} P_\ell(z)x^\ell\right)^2 dz = \int_{-1}^{1}(1-2xz+x^2)^{-1}\,dz$$
$$= x^{-1}[\ln(1+x)-\ln(1-x)] = \sum_{\ell=0}^{\infty}\frac{2}{2\ell+1}x^{2\ell}$$

while on the other hand, using the fact that for x small and $z \in (-1, 1)$ the convergence of $f(x, z)$ is uniform in z.

$$\int_{-1}^{1}\left(\sum_{\ell=0}^{\infty} x^\ell P_\ell(z)\right)^2 dz = \sum_{\ell=0}^{\infty}\left(\int_{-1}^{1} P_\ell(z)^2\,dz\right)x^{2\ell}$$

on account of the orthogonality relation.

(f) By the Stone–Weierstrass theorem, $\{z^\ell\}_{\ell=0}^{\infty}$ is a total set in $C(-1, 1)$ and so in $L^2(-1, 1)$. Thus, the set arrived at by applying the Gram–Schmidt procedure to $\{z^\ell\}_{\ell=0}^{\infty}$ is an orthonormal basis. But this basis is just $(-1)^\ell(\ell+\frac{1}{2})^{-1/2}P_\ell(z)$. ▮

It is a basic fact about power series that the interior of their region of convergence is always a circle. This follows from the fact that $(z'-z)^{-1} = \sum_{n=0}^{\infty} z^n/(z')^{n+1}$ converges in the region $|z| < |z'|$, that is, if z and z' can be separated by a circle with center at the origin. We want to find the natural regions of convergence for Legendre series, that is, series of the form $\sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(z)$. The functions that occur in the Legendre expansion for $(z'-z)^{-1}$ clearly play a critical role. We therefore define:

Definition The **associated Legendre functions** are defined in $\mathbb{C}\backslash[-1, 1]$ by

$$Q_\ell(z) = \frac{1}{2}\int_{-1}^{1}\frac{P_\ell(z')}{z-z'}\,dz'$$

The regions of convergence for Legendre series will be the interiors of certain curves:

Definition Let $z \in \mathbb{C}\backslash[-1, 1]$. By the **canonical ellipse through** z, we mean the unique ellipse passing through z with foci ± 1.

Theorem XI.63

(a) Let z and z' be given so that the canonical ellipse through z lies within the canonical ellipse through z'. Then

$$\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(z)Q_\ell(z')=(z'-z)^{-1} \tag{137}$$

The convergence of (137) is uniform as z and z' run respectively through compact sets C and D so long as there is a canonical ellipse E with C inside E and D outside E.

(b) If f is a function analytic in the interior of a canonical ellipse E, then the series

$$f(z)=\sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(z)$$

with

$$a_\ell=\frac{1}{2}\int_{-1}^{1}f(z)P_\ell(z)\,dz \tag{138}$$

converges uniformly on compact subsets of E.

(c) If a_ℓ is any sequence and the series $\sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(z)$ converges (respectively, diverges) for some $z_0\in\mathbb{C}\backslash[-1,1]$, then it converges absolutely for all z within the canonical ellipse through z_0 (respectively, diverges absolutely for all z outside the ellipse).

Proof (a) We first prove that the series (137) converges uniformly and then establish that the limit is indeed $(z'-z)^{-1}$. Consider the many to one map of $\mathbb{C}\to\mathbb{C}$ given by $\theta\mapsto z=\cos\theta$. The curves $\operatorname{Im}\theta=c$ go into canonical ellipses (Problem 90a); and given z fixed, $|\operatorname{Im}\theta|$ is independent of which $\theta=\cos^{-1}z$ is taken. Since $F(x,z)$ for z fixed has singularities at

$$x=z\pm\sqrt{z^2-1}=\cos\theta\pm i\sin\theta=e^{\pm i\theta}$$

we see that for z fixed, $F(x,z)$ has a radius of convergence $e^{-|\operatorname{Im}\theta|}$. By a Cauchy estimate, for any fixed $H>1$ and any compact C within the canonical ellipse $|\operatorname{Im}\theta|=\ln H$, $P_\ell(z)H^{-\ell}$ is uniformly bounded as z runs through C and ℓ through 0, 1, ... A similar estimate for $Q_\ell(z)$ (Problem 90b, c, d) shows that for any $H>1$ and D compact outside the canonical ellipse $|\operatorname{Im}\theta|=\ln H$, $Q_\ell(z)H^\ell$ is uniformly bounded as z runs through D. Given C, D, E as in the hypotheses, find ellipses E' (respectively, E'') given by $|\operatorname{Im}\theta|=\ln H'$ (respectively, $|\operatorname{Im}\theta|=\ln H''$) so that E' (respectively, E'') lies inside (respectively, outside) E and C (respectively, D) lies inside E'

(respectively, outside E''). Using the fact that $H'' > H'$, we see that for $z \in C$, $z' \in D$,

$$|P_\ell(z)Q_\ell(z')| \leq C[H'/H'']^\ell$$

so the series (137) converges.

If we fix E and z' outside E, then the limiting function $G(z, z')$ is analytic in z for z in E. Moreover,

$$\int_{-1}^{1} P_\ell(z)[G(z, z') - (z' - z)^{-1}]\, dz = 0$$

since $P_\ell(z)(\ell + \frac{1}{2})^{-1/2}$ is an orthonormal basis for $L^2[-1, 1]$. Thus $G(z, z') = (z' - z)^{-1}$ for $z \in (-1, 1)$ and so in all of E by analytic continuation.

(b) Given a compact C inside E, find another canonical ellipse E' so that C is inside E' and E' lies inside E. Then for $z \in C$, we have by the Cauchy theorem

$$f(z) = (2\pi i)^{-1} \oint_{E'} \frac{f(z')}{z' - z}\, dz' = \sum_{\ell=1}^{\infty} P_\ell(z) a_\ell (2\ell + 1)$$

where

$$a_\ell = \frac{1}{2\pi i} \oint_{E'} f(z')Q_\ell(z')\, dz'$$

and we have used the uniform convergence proven in (a). Since $P_\ell(z)$ is an orthogonal basis for $L^2(-1, 1)$, (138) holds.

(c) is left to the reader (Problem 91). ▌

Definition The **spherical Bessel functions** $j_\ell(x)$, $x \in \mathbb{C}$, are defined by

$$j_\ell(x) = \frac{e^{-i\pi\ell/2}}{2} \int_{-1}^{1} P_\ell(y) e^{ixy}\, dy$$

Theorem XI.64

(a) $j_\ell(x)$ is real for x real and $j_\ell(-x) = (-1)^\ell j_\ell(x)$.

(b) Each $j_\ell(x)$ is a finite linear combination of terms of the form $x^{-m} \cos x$ and $x^{-m} \sin x$ with $m \leq \ell + 1$.

(c) $j_\ell(x)$ is an entire function of x with $j_\ell(x) = O(x^\ell)$ for $x \to 0$.

(d) (Bessel's equation)

$$-\frac{d^2}{dx^2}[xj_\ell(x)] + \frac{\ell(\ell + 1)}{x^2}[xj_\ell(x)] = [xj_\ell(x)]$$

(e) $[xj_\ell(x) - \sin(x - \frac{1}{2}\pi\ell)] = O(x^{-1})$ as $x \to \infty$.
(f) If $\mathbf{e}$ is the unit vector $\langle 0, 0, 1\rangle$ and $\mathbf{r} \cdot \mathbf{e} = r\cos\theta$, then

$$e^{ik\mathbf{e}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} e^{i\pi\ell/2}(2\ell + 1)j_\ell(kr)P_\ell(\cos\theta)$$

where the series converges uniformly as k and $\mathbf{r}$ run through compact sets of $\mathbb{R}$ and $\mathbb{R}^3$ respectively.

Proof (a) $\overline{j_\ell(x)} = \frac{1}{2}e^{i\pi\ell}e^{-i\pi\ell/2}\int_{-1}^{1} P_\ell(y)e^{-ixy}\,dy$. Changing y into $-y$ and using $P_\ell(-y)e^{i\pi\ell} = P_\ell(y)$, we conclude that j_ℓ is real. Since P_ℓ is real,

$$j_\ell(-x)e^{+i\pi\ell/2} = \overline{j_\ell(x)e^{i\pi\ell/2}} = j_\ell(x)e^{-i\pi\ell/2}$$

or $j_\ell(-x) = (-1)^\ell j_\ell(x)$.

(b) Using $y^n e^{ixy} = (i^{-1}\,d/dx)^n e^{ixy}$, we see that

$$j_\ell(x) = e^{-i\pi\ell/2}P_\ell\left(\frac{1}{i}\frac{d}{dx}\right)\left[\frac{\sin x}{x}\right]$$

By induction, $(d/dx)^m x^{-1}\sin x$ is a finite linear combination of terms of the form $x^{-k}\sin x$ and $x^{-k}\cos x$ with $k \le m + 1$ so (b) follows.

(c) j_ℓ is the Fourier transform of a distribution of compact support and therefore an entire function of x. Moreover

$$\left.\frac{d^k j_\ell}{dx^k}\right|_{x=0} = \frac{1}{2}e^{-i\pi\ell/2}(i)^k\int_{-1}^{1} y^k P_\ell(y)\,dy$$

is zero if $k < \ell$ by the orthogonality relations for the Legendre polynomials. Thus $j_\ell(x) = O(x^\ell)$ as $x \to 0$.

(d) Let χ be the characteristic function of $(-1, 1)$ and let F be the distribution χP_ℓ. Then

$$\frac{dF}{dy} = \chi\frac{dP_\ell}{dy} + P_\ell(1)\,\delta(y - 1) - P_\ell(-1)\,\delta(y + 1)$$

so

$$(1 - y^2)\,\frac{dF}{dy} = \chi(1 - y^2)\,\frac{dP_\ell}{dy}$$

and thus

$$\begin{aligned}\frac{d}{dy}(1 - y^2)\frac{dF}{dy} &= \chi\frac{d}{dy}(1 - y^2)\frac{dP_\ell}{dy}\\ &= -\ell(\ell + 1)F\end{aligned}$$

by (d) of Theorem XI.62. Taking Fourier transforms,

$$x\left(1+\frac{d^2}{dx^2}\right)xj_\ell(x)=\ell(\ell+1)j_\ell(x)$$

which proves Bessel's equation.

(e) Since $e^{ixy}=(ix)^{-1}(d/dy)e^{ixy}$, integration by parts yields

$$j_\ell(x)=\frac{e^{-i\pi\ell/2}}{2}\frac{1}{ix}[e^{ix}P_\ell(1)-e^{-ix}P_\ell(-1)]-\frac{e^{-i\pi\ell/2}}{2ix}\int_{-1}^{1}e^{ixy}\frac{d}{dy}P_\ell(y)\,dy$$

By another integration by parts, one can see that the second term is $O(x^{-2})$ at infinity. Using $P_\ell(1)=1$, $P_\ell(-1)=(-1)^\ell$, the first term can be rewritten as $x^{-1}\sin(x-\frac{1}{2}\pi\ell)$.

(f) For k and r fixed, the function

$$f(r,k,\eta)=e^{ikr\eta}$$

is an entire function of η with uniform bounds as k, r, and η run through compact subsets of $\mathbb{R}$ (respectively, $\mathbb{C}$). Thus the Legendre series

$$f(r,k,\eta)=\sum_{\ell=0}^{\infty}(2\ell+1)a_\ell(k,r)P_\ell(\eta)$$

converges uniformly on such compact sets. Since

$$a_\ell(k,r)=\frac{1}{2}\int_{-1}^{1}P_\ell(\eta)f(r,k,\eta)\,d\eta$$

we see that $a_\ell(r)=e^{i\pi\ell/2}j_\ell(kr)$ by the definition of $j_\ell(x)$. ∎

Appendix 2 to XI.8: Jost solutions for oscillatory potentials

In this appendix and the next we shall consider certain classes of potentials with severe oscillations at infinity. To some extent, these examples are mathematical curiosities—but they are of theoretical interest for several reasons: First, these examples illuminate the modifications of the wave operators considered in Section 9; and secondly, there are connections with the phenomenon of positive eigenvalues (see Section XIII.13).

The net effort of these two appendices will be to show that so long as the average of V falls off, it does not matter that V fails to fall off. One can understand this heuristically in terms of the spreading of smooth free wave packets. Consider the following examples:

Example 1 Let

$$V(r) = (1 + r^2)^{-1} e^r \sin(e^r) \tag{139}$$

V is clearly very singular at infinity. But its average is not since an integration by parts shows that

$$\int_r^R V(x)\, dx$$

$$= (1 + r^2)^{-1} \cos(e^r) - (1 + R^2)^{-1} \cos(e^R) + 2 \int_r^R x(1 + x^2)^{-2} \cos(e^x)\, dx$$

so that

$$W(r) = -\lim_{R \to \infty} \int_r^R V(x)\, dx \tag{140}$$

exists and is "short-range" in the sense that

$$|W(r)| \le C(1 + r^2)^{-1}$$

Because of this falloff of the average of V, it turns out that $-\Delta + V$ can be defined as a sum of forms and that it is bounded from below in spite of the fact that V is so unbounded. For $V(r) = \partial W/\partial r$ and thus on $\mathbb{R}^n$

$$V(x) = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} G_i(\mathbf{x}) + K(x)$$

where $G_i(\mathbf{x}) = x^{-1} x_i W(x)$ and $K(x) = -(n - 1)x^{-1} W(x)$. On the basis of this we claim that for any ε, there is a C_ε with

$$(\varphi, V\varphi) \le \varepsilon(\varphi, (-\Delta)\varphi) + C_\varepsilon(\varphi, \varphi) \tag{141}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. K is $-\Delta$-form bounded with relative bound zero. Moreover, by an integration by parts followed by the Schwarz inequality,

$$|(\varphi, (\partial G_i/\partial x_i)\varphi)| = \left| \int \frac{\partial G_i}{\partial x_i} |\varphi|^2\, dx \right| = 2|\mathrm{Re}(\varphi, G_i\, \partial\varphi/\partial x_i)|$$

$$\le (\varphi, G_i^2 \varphi)^{1/2} (\partial\varphi/\partial x_i, \partial\varphi/\partial x_i)^{1/2}$$

so that (141) follows since G_i^2 is $-\Delta$-form bounded with relative bound zero. From (141), $(\varphi, V\varphi)$ can be extended to $Q(-\Delta)$ and $-\Delta + V$ is a semibounded closed quadratic form on $Q(-\Delta)$. We warn the reader that for arbitrary $\varphi \in Q(-\Delta)$, it may *not* be true that $\int |V(x)|\, |\varphi(x)|^2\, dx < \infty$; $(\varphi, V\varphi)$ is defined via a limiting argument. One can actually develop a scattering theory for $-\Delta + V$ by mimicking the ideas in Theorem XI.31 (see Problem 92) or the methods of Section XIII.8 (see the reference in the Notes). Here we want to consider Jost functions for such V's.

Example 2 Let

$$V(r) = \sum_{j=1}^{m} \gamma_j r^{-1} \sin(\alpha_j r) + Q(r) \tag{142a}$$

with

$$|Q(r)| \le C(1 + r^2)^{-\frac{1}{2}-\varepsilon} \tag{142b}$$

for some $\varepsilon > 0$ and C. In this case V is bounded, so there is no problem defining $-\Delta + V$. Two subtle phenomena are associated with $-\Delta + V$. In the first place, there is a potential of the form (142) so that $(-\Delta + V)\varphi = \varphi$ has a square integrable solution even though $V \to 0$ at infinity. (See Example 1 of Section XIII.13 and the discussion there.) In the second place, $V(r)$ does not fit into the framework of potentials whose scattering theory we have developed since $\int_1^\infty |V(r)|\, dr = \infty$. In Section 9 we shall develop a modified scattering theory for potentials like the Coulomb potential. Unfortunately, the estimates needed to make the Coulomb theory work are not applicable to potentials of the form of (142). However, that theory suggests the type of scattering theory one might expect for potentials of this form. In Section 9 we make a modification of the free dynamics in defining time-dependent wave operators. As $t \to \infty$, this modification diverges in the Coulomb case, and so without it the wave operators do not exist. Because the indefinite integral (140) exists if V obeys (142), the modification of Section 9 actually converges in this case; so if the modified wave operators exist, so do the original wave operators. This suggests that the ordinary wave operators exist for this case. By investigating Jost solutions for these potentials we shall see when positive eigenvalues exist and also develop the scattering theory. This scattering theory appears in the next appendix.

Since we are here interested in the problems associated with oscillations at infinity, we shall suppose throughout this appendix that $V(r)$ is continuous and locally bounded. Our methods can be easily modified to accommodate local singularities in V. In understanding Examples 1 and 2, the following result is needed; it and its corollaries are easily extended to the case where X is a Banach space. In our applications, $\dim X = 2$.

Proposition Let X be a finite-dimensional normed vector space. Let $C(x)$ be a continuous function on $[R_0, \infty)$ with values in $\mathscr{L}(X)$. Let $D(x, y)$

be a measurable function on $Q \equiv \{\langle x, y\rangle \mid R_0 \le x \le y < \infty\}$ with values in $\mathscr{L}(X)$.

(a) Suppose that

$$\gamma \equiv \sup_{x \ge R_0} \|C(x)\| + \sup_{x \ge R_0} \int_x^\infty \|D(x, y)\|\, dy < 1$$

Then, for any $u_0 \in X$, the equation

$$u(x) = u_0 + C(x)u(x) + \int_x^\infty D(x, y)u(y)\, dy \tag{143}$$

has a unique solution in $L^\infty(R_0, \infty)$. Furthermore, this solution is continuous.

(b) Moreover, if

$$\gamma(r) \equiv \sup_{x \ge r} \|C(x)\| + \sup_{x \ge r} \int_x^\infty \|D(x, y)\|\, dy$$

goes to zero as $r \to \infty$, then $\lim_{x\to\infty} u(x) = u_0$ and for $x > R_0$,

$$\|u(x) - u_0\| \le \gamma(x)[1 - \gamma(x)]^{-1}\|u_0\|$$

(c) Suppose that C is continuously differentiable, that D is continuous on Q, and that for each fixed x,

$$f_\varepsilon(y) = \varepsilon^{-1}[D(x + \varepsilon, y) - D(x, y)]$$

converges in $L^1(\mathbb{R}, \infty)$ to a function, denoted by $\partial D/\partial x$, which is continuous in x in L^1 sense. Then the solution u of (143) is continuously differentiable and

$$u'(x) = C'(x)u(x) + C(x)u'(x) - D(x, x)u(x) + \int_x^\infty \frac{\partial D}{\partial x}(x, y)u(y)\, dy \tag{144}$$

(a) and (b) remain true if the constant u_0 is replaced by a continuous function $u_0(x)$ with $\sup_{x \ge R_0} \|u_0(x)\| = Q_0 < \infty$ so long as $\|u_0\|$ is replaced by Q_0 in all estimates. (c) still holds in this case so long as $u_0(x)$ is C^1 and a term $u_0'(x)$ is added on the right side of (144).

Proof (a) Define $u_n(x)$ inductively by $u_0(x) = u_0$ and

$$u_n(x) = C(x)u_{n-1}(x) + \int_x^\infty D(x, y)u_{n-1}(y)\, dy$$

One easily proves inductively that $u_n(x)$ is continuous and

$$\sup_{|x| \ge r} \|u_n(x)\| \le \gamma(r)^n \|u_0\| \tag{145}$$

Since $\gamma(R_0) = \gamma < 1$, $\sum_{n=0}^{N} u_n(x)$ converges uniformly to a continuous function $u(x)$ that obeys (143). If v is any solution of (143) in $L^\infty(R_0, \infty)$, by iterating (143), one finds that

$$\left\| v - \sum_{n=0}^{N} u_n(x) \right\| \leq \gamma^{N+1} \|v\|_\infty$$

so taking $N \to \infty$, $v = u$.

(b) By (145),

$$\|u - u_0\| \leq \sum_{n=1}^{\infty} \gamma(r)^n \|u_0\| = \gamma(r)(1 - \gamma(r))^{-1} \|u_0\|$$

(c) Under the hypothesis, u_n is inductively seen to be continuously differentiable with

$$u_n'(x) = C'(x)u_{n-1}(x) + C(x)u_{n-1}'(x) - D(x, x)u_{n-1}(x) + \int_x^\infty \frac{\partial D}{\partial x}(x, y)u_{n-1}(y)\,dy$$

Using (145), one can prove (Problem 93) the following bounds inductively:

$$|u_n'(x)| \leq n\gamma^n \|u_0\| A(x), \qquad x \geq R_0$$

where

$$A(x) = \gamma^{-1}\left(\|C'(x)\| + \|D(x, x)\| + \int_x^\infty \left\| \frac{\partial D}{\partial x}(x, y) \right\| dy \right)$$

It follows that $\sum_{n=0}^{\infty} u_n'(x)$ converges uniformly on any compact subset of $[R_0, \infty)$, so that $u(x)$ is differentiable with derivative $\sum_{n=0}^{\infty} u_n'(x)$. Thus (144) holds. The case when u_0 is x-dependent is left to the reader (Problem 93). ∎

Theorem XI.65 Let $A(x)$ be a continuous function from $[R_0, \infty)$ to $\mathscr{L}(X)$, the bounded operators on a finite-dimensional normed linear space. Assume that $\|A(x)\| \in L^1(R, \infty)$. Suppose that $u_0 \in X$. Then there exists a unique continuously differentiable function $u(x, u_0)$ so that

$$\frac{du}{dx} = A(x)u(x)$$

and $\lim_{x\to\infty} u(x) = u_0$. Every nonzero solution has a nonzero limit as $x \to \infty$. Moreover, $\|u(x) - u_0\| \leq 2\|u_0\| \int_x^\infty \|A(y)\|\,dy$ for all x with $\int_x^\infty \|A(y)\|\,dy < \frac{1}{2}$.

Proof Pick R_1 so that $\int_{R_1}^{\infty} \|A(x)\| \, dx < 1$. Then, by the proposition,

$$u(x) = u_0 - \int_x^{\infty} A(y)u(y) \, dy$$

has a unique solution on $[R_1, \infty)$ that is continuously differentiable with $u'(x) = A(x)u(x)$. Using local existence and uniqueness, this can be continued to $[R, \infty)$. Picking a basis for X, we can find n linearly independent solutions with different linearly independent limits at infinity. By local uniqueness, these span all solutions yielding uniqueness together with the fact that every solution has a limit. The last bound follows from (b) of the proposition. ∎

Example 3 Consider the equation

$$-\varphi''(x) + V(x)\varphi(x) = k^2\varphi(x)$$

on $[1, \infty)$ where $\int_1^{\infty} |V(x)| \, dx < \infty$. Let $\Psi(x) = \binom{\varphi(x)}{\varphi'(x)}$. Then $\Psi'(x) = C(x)\Psi(x)$ where

$$C(x) = \begin{pmatrix} 0 & 1 \\ V(x) - k^2 & 0 \end{pmatrix}$$

Let $\varphi_{\pm}$ be the vector valued functions

$$\varphi_{\pm}(x) = \begin{pmatrix} e^{\pm ikx} \\ \pm ike^{\pm ikx} \end{pmatrix}$$

and write $\Psi(x) = \alpha(x)\varphi_{+}(x) + \beta(x)\varphi_{-}(x)$ where α and β are complex-valued functions. Then $q = \binom{\alpha}{\beta}$ obeys $q(x) = M(x)\Psi(x)$ with

$$M(x) = (2ik)^{-1}\begin{pmatrix} ike^{-ikx} & e^{-ikx} \\ ike^{ikx} & -e^{ikx} \end{pmatrix}$$

Thus

$$q'(x) = D(x)q(x) \tag{146a}$$

where $D(x) = M'(x)M(x)^{-1} + M(x)C(x)M(x)^{-1}$ so

$$D(x) = (2ik)^{-1}V(x)\begin{pmatrix} 1 & e^{-2ikx} \\ -e^{2ikx} & -1 \end{pmatrix} \tag{146b}$$

Applying Theorem XI.65 to (146), we see that if $\int_1^{\infty} |V(x)| \, dx < \infty$, then (146) has solutions asymptotic to any q_0 as $x \to \infty$. Taking $q = \binom{1}{0}$, we find a solution φ of the Schrödinger equation with $|\varphi(x) - e^{ikx}| + |\varphi'(x) - ike^{ikx}| \to 0$ as $x \to \infty$. We thus have a proof of the existence of Jost solutions somewhat independent of the one given in the section.

Example 4 Consider solutions of $-f''(r) + \ell(\ell + 1)r^{-2}f(r) = k^2 f(r)$. Proceeding as in the above example, one can show that any real-valued solution obeys $|f(r) - C \sin(kr + D)| = O(r^{-1})$ and in particular

$$|krj_\ell(kr) - \sin(kr - \tfrac{1}{2}\pi\ell)| = O(r^{-1})$$

To handle Example 2, we need an interesting extension of Theorem XI.65.

Theorem XI.66 (Dollard–Friedman theorem) Let $A(x)$ be a continuous function from $[R, \infty)$ to $\mathscr{L}(X)$, the bounded operators on a finite-dimensional normed linear space. Suppose that $A = A_1 + A_2$ where

(i) $\|A_1(\cdot)\| \in L^1(R, \infty)$.
(ii) $B(x) = -\lim_{r\to\infty} \int_x^r A_2(y)\,dy$ exists.
(iii) $\|B(\cdot)A(\cdot)\| \in L^1(R, \infty)$.

Then there exists a unique continuously differentiable X-valued function $u(x; u_0)$ such that

$$\frac{du}{dx} = A(x)u(x)$$

and $\lim_{x\to\infty} u(x; u_0) = u_0$. Every nonzero solution of the differential equation has a nonzero limit as $x \to \infty$ and

$$\begin{aligned} &|u(x; u_0) - u_0| \\ &\quad \le 2\left(\sup_{y \ge x} \|B(y)\| + \int_x^\infty \|A_1(y)\|\,dy + \int_x^\infty \|B(y)A(y)\|\,dy\right)\|u_0\| \end{aligned} \tag{147}$$

for all x such that the expression in ( ) is smaller than $\frac{1}{2}$.

Proof We begin with some manipulation of the formal equation

$$u(x) = u_0 - \int_x^\infty A(y)u(y)\,dy$$

Write $A_2(y) = dB(y)/dy$ and integrate by parts. The boundary term at infinity should vanish since

$$\lim_{y\to\infty} \|B(y)\| = 0 \tag{148}$$

on account of the convergence of the integral defining $B(y)$. Using $u'(y) = A(y)u(y)$, we find that

$$u(x) = u_0 + B(x)u(x) - \int_x^\infty [A_1(y) - B(y)A(y)]u(y)\,dy \tag{149}$$

Having arrived at (149) formally, we solve it and then show that the solution has the required properties.

Let

$$\gamma(x) = \sup_{y \geq x} \|B(y)\| + \int_x^\infty (\|A_1(y)\| + \|B(y)A(y)\|)\,dy$$

By (148) and the hypotheses, $\gamma(x) \to 0$ as $x \to \infty$; so, by the proposition, (149) has solutions in $[R_1, \infty)$ for R_1 sufficiently large and the solutions obey (147). By (c) of the proposition, the solution is C^1 and

$$u'(x) = B(x)u'(x) + A_2(x)u(x) + [A_1(x) - B(x)A(x)]u(x)$$

so that

$$(1 - B(x))u'(x) = (1 - B(x))A(x)u(x)$$

By (148), $1 - B(x)$ is invertible for x large; thus, we have the desired solution of the differential equation for x large. The rest of the proof follows by local solvability as in Theorem XI.65. ▮

Example 2, revisited We seek solutions of $-\varphi''(x) + V(x)\varphi(x) = k^2\varphi(x)$ where $V(x)$ has the form of (142). As in Example 3, we begin by writing the equation in the form of (146). Write $D = D_1 + D_2$ where D_1 comes from the $Q(x)$ term and D_2 from the $r^{-1}\sin(\alpha_j r)$ terms. D_1 is clearly in L^1. Moreover, since

$$\int_r^x y^{-1}e^{i\beta y}\,dr = (i\beta y)^{-1}e^{i\beta y}\Big]_r^x + (i\beta)^{-1}\int_r^x y^{-2}e^{i\beta y}\,dy$$

we see that for $\beta \neq 0$, $\lim_{x\to\infty} \int_r^x y^{-1}e^{i\beta y}\,dy$ exists and the resulting function is bounded by r^{-1}. It follows that, so long as $\alpha_j \neq \pm 2k$ for all j, $B(r) = \int_r^\infty D_2(x)\,dx$ exists as an improper integral, and $BD \in L^1$ with $\int_r^\infty \|B(y)D(y)\|\,dy = O(r^{-1})$. As a result, Theorem XI.66 is applicable and immediately yields a proof of (a) and (b) of the following theorem.

Theorem XI.67 Let V have the form of (142).

(a) Let k be a real number with $k \neq 0, \pm\frac{1}{2}\alpha_1, \ldots, \pm\frac{1}{2}\alpha_m$. Then every nonzero solution of $-\varphi'' + V\varphi = k^2\varphi$ satisfies

$$\lim_{x\to\infty} [\varphi(x) - ae^{ikx} - be^{-ikx}] = 0$$

for suitable a and b. In particular, $-\varphi'' + V\varphi = k^2\varphi$ has no nonzero square integrable solutions.

(b) For any k as in (a), there exists a unique solution $\varphi(x; k)$ of $-\varphi'' + V\varphi = k^2\varphi$ on $[1, \infty)$ satisfying

$$|\varphi(x; k) - e^{-ikx}| \leq c_k |x|^{-\alpha}, \qquad x \geq 1$$

with $\alpha = \min\{1, 2\varepsilon\}$ where ε is given in (142b). Moreover, c_k can be chosen independently of k as k runs through a compact subset of $\{k \in \mathbb{R} \,|\, k \neq 0, \pm\frac{1}{2}\alpha_1, \ldots, \pm\frac{1}{2}\alpha_m\}$.

(c) Suppose that $k = \frac{1}{2}\alpha_j$ for some j. Then there exists a solution u of $-\varphi'' + V\varphi = k^2\varphi$ that satisfies

$$u = \begin{cases} r^{-\gamma_j/2\alpha_j}(\cos(\frac{1}{2}\alpha_j r) + o(1)), & \gamma_j/\alpha_j > 0 \\ r^{+\gamma_j/2\alpha_j}(\sin(\frac{1}{2}\alpha_j r) + o(1)), & \gamma_j/\alpha_j < 0 \end{cases}$$

For a proof of part (c), see the reference in the Notes and Problems 97 and 98. The point of part (c) is that when γ_j is bigger than α_j, there is a solution of the Schrödinger equation that is square integrable at ∞. In general, if one has a one-parameter family of such potentials, one of the solutions will obey the requisite boundary conditions at the origin. Therefore, there exist Schrödinger operators with positive eigenvalues embedded in the continuous spectrum. This is further discussed in Section XIII.13.

In the next appendix we shall see that so long as $\varepsilon > \frac{1}{4}$, part (b) of the theorem can be used to prove that $\Omega^{\pm}(-\Delta + V, -\Delta)$ exist and have equal ranges.

The proof of the Dollard–Friedman theorem and the solution of the problem posed in Example 2 involved integration by parts in the obvious integral equation. The same method works in Example 1, but the "suitable equation" is not given directly by (146) but rather by the Jost integral equation (126). We remark that one can "derive" the Jost equation easily from (146).

Example 1, revisited We begin with the Jost equation and formally manipulate under the assumption that $V(r) = \partial W/\partial r$ with

$\int_x^\infty |W(r)|\,dr < \infty$. Integrating by parts in

$$\varphi(x) = e^{-ikx} - \int_x^\infty \frac{\sin k(x-y)}{k} V(y)\varphi(y)\,dy$$

and dropping the boundary term at infinity, we obtain

$$\varphi(x) = e^{-ikx} - \int_x^\infty W(y)[\cos(kx-ky)\varphi(y) - k^{-1}\sin(kx-ky)\varphi'(y)]\,dy \tag{150a}$$

and similarly, integrating by parts in

$$\varphi'(x) = -ike^{-ikx} - \int_x^\infty \cos(kx-ky)V(y)\varphi(y)\,dy$$

we obtain

$$\begin{aligned}\varphi'(x) = {} & -ike^{-ikx} + W(y)\varphi(y) \\ & + \int_x^\infty W(y)[k\sin(kx-ky)\varphi(y) + \cos(kx-ky)\varphi'(y)]\,dy \end{aligned}\tag{150b}$$

Rewriting (150) as a system of equations for $\langle\varphi, \varphi'\rangle$, we see that it has a C^1 solution on account of the proposition. Using part (c) of the proposition, one easily sees that the resulting solution obeys $\varphi''(x) = V(x)\varphi(x) - k^2\varphi(x)$. We summarize with:

Theorem XI.68 Let $V(r)$ be a continuous function with $V(r) = \partial W/\partial r$ where $W \in L^1[1, \infty)$. Then:

(a) $-\varphi'' + V\varphi = k^2\varphi$ has no nonzero square integrable solution for $k \neq 0$.

(b) Suppose that $|W(x)| \leq C|x|^{-1-\varepsilon}$. Then, for any $k \neq 0$, there is a solution $\varphi(x; k)$ of $-\varphi'' + V\varphi = k^2\varphi$ in $[1, \infty)$ with

$$|\varphi(x, k) - e^{-ikx}| \leq c(k)|x|^{-\varepsilon}, \qquad x \geq 1$$

$c(k)$ can be chosen independently of k for $|k| \geq k_0 > 0$.

Appendix 3 to XI.8: Jost solutions and the fundamental problems of scattering theory

In this appendix we consider cases where one has regular solutions of the Schrödinger equation $u_\ell(x; k)$ and good control on how fast $|u_\ell(x; k) - \sin(kx - \frac{1}{2}\ell\pi + \delta_\ell)|$ goes to zero as $|x|$ goes to ∞. From this information we shall prove that $\Omega^\pm$ exist, that $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ and that S is multiplication by $e^{2i\delta_\ell(k)}$ in the representation where energy and angular momentum are diagonal. This will enable us to recover some of the results of the section and more importantly to develop scattering theory for some of the potentials of Appendix 2. Moreover, it will shed some light on the invariance principle for wave operators. Throughout, we use the symbol $\hat{x}$ for $\mathbf{x}/|x|$. The basic result is:

Theorem XI.69 Let $V(\mathbf{x})$ be a central potential on $\mathbb{R}^3$ so that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Suppose that for each $\ell = 0, 1, \ldots,$ there is a closed set $\mathscr{E}_\ell$ of measure zero in $(0, \infty)$ such that for each $k \in (0, \infty)\backslash\mathscr{E}_\ell$, there is a real-valued distributional solution

$$\varphi(\mathbf{x}; k) = (k|\mathbf{x}|)^{-1} u_\ell(|\mathbf{x}|; k) Y_{\ell m}(\hat{x})$$

of $(-\Delta + V)\varphi_\ell = k^2\varphi_\ell$ obeying

$$|u_\ell(k, r) - \sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell(k))| \le c_\ell(k)(1 + |r|)^{-\frac{1}{2}-\gamma} \tag{151}$$

for a fixed $\gamma > 0$. Suppose that $\varphi_\ell(\mathbf{x}; \cdot)$ and $\delta_\ell(\cdot)$ are measurable and that $\sup_{k\in K} c_\ell(k) < \infty$ for every compact subset K of $(0, \infty)\backslash\mathscr{E}_\ell$. Then, $\Omega^\pm(-\Delta + V, -\Delta)$ exist, $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$, and $S = (\Omega^-)^*\Omega^+$ is given by

$$S\left[\sum_{\ell, m} Y_{\ell m}(\hat{x}) \int_0^\infty j_\ell(k|x|) f_{\ell m}(k)\, dk\right] = \sum_{\ell, m} Y_{\ell m}(\hat{x}) \int_0^\infty j_\ell(k|x|) e^{2i\delta_\ell(k)} f_{\ell m}(k)\, dk \tag{152}$$

Proof Fix ℓ, m, and $f \in C_0^\infty((0, \infty)\backslash\mathscr{E}_\ell)$. Let

$$\psi(\mathbf{x}) = Y_{\ell m}(\hat{x}) \int_0^\infty (kx)^{-1} u_\ell(x; k) f(k)\, dk$$

$$\psi_\pm^{(0)}(\mathbf{x}) = Y_{\ell m}(\hat{x}) \int_0^\infty j_\ell(kx) e^{\mp i\delta_\ell(k)} f(k)\, dk$$

Using (151) and $f \in C_0^\infty$, one easily sees that ψ and $\psi_\pm^{(0)}$ are in $L^2(\mathbb{R}^3)$ (Problem 94). We shall show that

$$\lim_{t\to\mp\infty} \|e^{-itH}\psi - e^{-itH_0}\psi_\pm^{(0)}\| = 0 \tag{153}$$

Once (153) is proven, we conclude that $\Omega^\pm$ exist for a dense set and obtain formulas for $\Omega^\pm$ that establish $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ and that (152) holds. Let C be complex conjugation. Then $e^{-itH_0}C = Ce^{itH_0}$ and $e^{-itH}C = Ce^{itH}$, so (153) need only be proven for the case $t \to -\infty$.

Since $-\Delta + V = H$ obeys $H\varphi_\ell(\cdot\,; k) = k^2\varphi_\ell(\cdot\,; k)$ in distributional sense, we see that for $\eta \in C_0^\infty(\mathbb{R}^3)$,

$$(H\eta, \psi) = (\eta, \tilde{\psi})$$

where $\tilde{\psi}$ is given by the formula for ψ except that $f(k)$ is replaced by $k^2 f(k)$. Since H is essentially self-adjoint on C_0^∞, $\psi \in D(H)$ and $H\psi = \tilde{\psi}$. Repeating this and using the fact that $f \in C_0^\infty$, we see that

$$\psi(\mathbf{x}, t) \equiv (e^{-itH}\psi)(\mathbf{x}) = Y_{\ell m}(\hat{\mathbf{x}}) \int_0^\infty (kx)^{-1} u_\ell(x; k) e^{-itk^2} f(k)\, dk$$

Similarly,

$$\psi_+^{(0)}(\mathbf{x}, t) \equiv (e^{-itH_0}\psi)(\mathbf{x}) = Y_{\ell m}(\hat{\mathbf{x}}) \int_0^\infty j_\ell(kx) e^{-itk^2} e^{-i\delta_\ell(k)} f(k)\, dk$$

Now, *define* $\eta(\mathbf{x}, t)$ by

$$\eta(\mathbf{x}, t) = Y_{\ell m}(\hat{\mathbf{x}}) \int_0^\infty (kx)^{-1} \sin(kx - \tfrac{1}{2}\ell\pi + \delta_\ell(k)) e^{-itk^2} f(k)\, dk$$

Then

$$\alpha_t(\mathbf{x}) \equiv |\psi(\mathbf{x}, t) - \eta(\mathbf{x}, t)| = |Y_{\ell m}(\hat{\mathbf{x}})| \left| \int_0^\infty (kx)^{-1} q(x, k) e^{-itk^2} f(k)\, dk \right|$$

where $q(x, k) = u(x; k) - \sin(kx - \frac{1}{2}\ell\pi + \delta_\ell(k))$. Now, for each fixed x, $(kx)^{-1}q(x, k)f(k)$ is in $L^1(0, \infty)$ as a function of k by (151), so $\alpha_t(x) \to 0$ as $t \to \pm\infty$ by the Riemann–Lebesgue lemma. Moreover, by (151),

$$|\alpha_t(\mathbf{x})| \le C\, |Y_{\ell m}(\hat{\mathbf{x}})|\, x^{-1}(1 + x)^{-\frac{1}{2}-\gamma}$$

for all t. Thus, by the dominated convergence theorem, $\int |\alpha_t(x)|^2\, d^3x \to 0$ as $t \to \pm\infty$. This reduces the proof of (153) to showing that

$$\int |\psi_+^{(0)}(x, t) - \eta(x, t)|^2\, d^3x \to 0 \qquad \text{as} \quad t \to -\infty$$

Let

$$\zeta_\pm(\mathbf{x}, t) = Y_{\ell m}(\hat{\mathbf{x}}) \int (kx)^{-1} e^{\pm ikx} e^{\pm i\delta_\ell(k)} e^{\mp i\ell\pi/2} e^{-ik^2 t} f(k)\, dk$$

By Lemma 3 of Section 3,

$$\lim_{t \to -\infty} \int |\zeta_+(\mathbf{x}, t)|^2\, d^3x = 0$$

so

$$\lim_{t\to-\infty} \int |\eta(\mathbf{x}, t) - \tfrac{1}{2}i\zeta_-(\mathbf{x}, t)|^2 \, d^3x = 0$$

The same set of arguments we have just made leads to

$$\lim_{t\to-\infty} \int |\psi_+^{(0)}(\mathbf{x}, t) - \tfrac{1}{2}i\zeta_-(\mathbf{x}, t)|^2 \, d^3x = 0$$

if we use $|krj_\ell(kr) - \sin(kr - \frac{1}{2}\ell\pi)| \le C(k)(1 + |r|)^{-1}$ in place of (151). We conclude that (153) holds. ▌

In the above, φ was a generalized eigenfunction with eigenvalue $E(k) = k^2$. The exact functional form of $E(k)$ played no role in the proof, which goes through as long as E is strictly monotone. This not only demonstrates that an invariance principle holds in the context of the above theorem, but makes transparent the reason that invariance holds at all.

Corollary 1 If $V(\mathbf{x})$ is a central potential satisfying

$$|V(x)| \le C(1 + |x|)^{-\frac{3}{2}-\varepsilon}$$

($\varepsilon > 0$), then $\Omega^\pm(-\Delta + V, -\Delta)$ exist, $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$, and the S-operator is given by (152).

Of course, this result is not a new one for us—stronger results are proven in Section 8—but the proof is quite direct. The following result is based on Theorem XI.67.

Corollary 2 Let

$$V(x) = \sum_{j=1}^{m} \gamma_j r^{-1} \sin(\alpha_j r) + Q(r)$$

with $|Q(r)| \le C(1 + r)^{-\frac{3}{2}-\varepsilon}$. Then $\Omega^\pm(-\Delta + V, -\Delta)$ exist, $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ and the S-operator is given by (152).

By modifying the arguments slightly, one can accommodate some of the highly oscillatory potentials of Theorem XI.68 (Problem 95). Moreover, by appealing to results from the theory of ordinary differential equations, one can prove that $\operatorname{Ran}\Omega^\pm = \operatorname{Ran} P_{\mathrm{ac}}(-\Delta + V)$ and that $-\Delta + V$ has no singular continuous spectrum in the situations described by Corollaries 1 and 2. Finally, we note a version of Theorem XI.69 for noncentral potentials.

Theorem XI.70 Let $V(\mathbf{x})$ be a measurable function on $\mathbb{R}^3$ so that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Suppose that there is a closed set $\mathscr{E}$ of measure zero in $\mathbb{R}^3$, so that for each $\mathbf{k} \in \mathbb{R}^3 \backslash \mathscr{E}$, there is a distributional solution $\varphi(\mathbf{x}, \mathbf{k})$ of $(-\Delta + V)\varphi = k^2\varphi$ obeying

$$|\varphi(\mathbf{x}, \mathbf{k}) - e^{i\mathbf{k}\cdot\mathbf{x}} - \gamma(\mathbf{k}, \hat{x})x^{-1}e^{ikx}| \leq C(\mathbf{k})(1 + x)^{-\frac{3}{2}-\varepsilon} \tag{154}$$

for $|x| \geq 1$. Suppose that φ and γ are measurable functions, that $\overline{\varphi(\mathbf{x}, \mathbf{k})} = \varphi(\mathbf{x}, -\mathbf{k})$, and that $\sup_{\mathbf{k}\in K} |C(\mathbf{k})| < \infty$ for every compact subset $K \subset \mathbb{R}^3 \backslash (\mathscr{E} \cup \{0\})$. Then $\Omega^\pm$ exist, $\operatorname{Ran} \Omega^+ = \operatorname{Ran} \Omega^-$, and $S = (\Omega^-)^*\Omega^+$ is given by

$$(Sf)(x) = f(x) + \int_{\omega\in S^2} \int \beta(k, \Omega)\hat{f}(|\mathbf{k}|\omega)e^{+i\mathbf{k}\cdot\mathbf{x}}\, d^3k\, d\Omega(\omega)$$

where

$$\beta(k, \Omega) = i\pi^{-1}\gamma(k, \Omega)$$

The details of the proof, which are very similar to those of Theorem XI.69, are left to the reader (Problem 96). However, since the proof provides such a graphic picture of scattering and one which is so similar to that in certain physics textbook presentations, we sketch some of the intermediate steps. Let $g \in C_0^\infty(\mathbb{R}^3 \backslash (\mathscr{E} \cup \{0\}))$ and

$$\psi(\mathbf{x}) = \int g(\mathbf{k})\varphi(\mathbf{x}, \mathbf{k})\, d^3k$$

Then, as in the central case,

$$(e^{-iHt}\psi)(\mathbf{x}) = \int g(\mathbf{k})e^{-ik^2t}\varphi(\mathbf{x}, \mathbf{k})\, d^3k$$

By (154) and the dominated convergence theorem, $\|e^{-itH}\psi - \eta_t\| \to 0$ as $t \to \pm\infty$ where

$$\eta_t(\mathbf{x}) = \int g(\mathbf{k})e^{-ik^2t}[e^{i\mathbf{k}\cdot\mathbf{x}} - \gamma(\mathbf{k}, \hat{x})x^{-1}e^{ikx}]\, d^3k$$

The point is that as $t \to -\infty$, the second term goes to zero by an extension of Lemma 3 of Section 3 so that $\|e^{-itH}\psi - e^{-itH_0}[(2\pi)^{3/2}\check{g}]\| \to 0$ as $t \to -\infty$. As $t \to +\infty$, both terms contribute, and we have both the original wave and a "scattered" wave.

XI.9 Long-range potentials

Both the classical and quantum-mechanical scattering theories that we have developed depend on estimates whose proofs break down when the potentials have r^{-1} falloff. From what we have done so far, it is not clear whether the results could be pushed through for long range potentials with more work on the estimates, but one consequence of what we do in this section is that, in fact, the unmodified theories do not extend further; for example, using Theorem XI.71 below, one can prove (Problem 99) that

$$\operatorname*{w-lim}_{t\to\pm\infty} e^{it(-\Delta-r^{-1})}e^{it\Delta} = 0 \tag{155}$$

so that the strong limit does not exist.

In this section we shall first discuss briefly the classical and quantum Coulomb problems and then systematically develop the general long-range case.

At first sight, the scattering theory for classical Coulomb forces seems to be in fine shape. The solutions of

$$\ddot{\mathbf{r}} = -r^{-2}(\mathbf{r}/r)$$

are well known in closed form. The quantities $\ell = \dot{\mathbf{r}} \times \mathbf{r}$ and $E = \frac{1}{2}|\dot{\mathbf{r}}|^2 - r^{-1}$ are conserved. Picking polar coordinates in the plane orthogonal to ℓ, the orbits are given by

$$r(\theta)^{-1} = \ell^{-2}[1 + \sqrt{1 + E\ell^2}\cos(\theta - \theta_0)]$$

This describes an ellipse (or circle) if $E < 0$, a parabola if $E = 0$, and one branch of a hyperbola if $E > 0$. The hyperbolic orbits are clearly the ones one should try to associate with a scattering theory. There are straight line asymptotes to the hyperbolas, which means that the orbit in x space is asymptotic to free orbits. Moreover, the velocity clearly has a limiting direction as $t \to \pm\infty$ and by the fact that $r \to \infty$ and $v = \sqrt{2E + 2r^{-1}}$, it has a limiting magnitude also. Thus the *orbit* in phase space is asymptotic to a free orbit. The problem is with the time parametrization of these orbits. Free orbits have $\mathbf{r}_{\text{free}}(t) = \mathbf{c}t + \mathbf{b} + o(1)$. On the other hand, since $\dot{\mathbf{r}}$ has a limit in the interacting case

$$r(t) = \mathbf{c}t + o(t)$$

as $t \to \infty$. We can further analyze the $o(t)$ term in this expansion by using

$$\frac{1}{\sqrt{2}}\left|\frac{dr}{dt}\right| = \sqrt{E + r^{-1}} = \sqrt{E}(1 + (2E)^{-1}(ct)^{-1} + o(t^{-1}))$$

to obtain

$$\mathbf{r}(t) = \mathbf{c}t + \mathbf{d} \ln t + O(1)$$

as $t \to \infty$. This makes it clear that the Coulomb orbits $r(t)$ do not approach $\mathbf{a} + \mathbf{b}t$, but nevertheless the occurrence of asymptotes suggests strongly that some kind of modified scattering theory should work. There is a logarithmic slippage of the physical time parametrization of the Coulomb orbit relative to the physical time parametrization of the free asymptote. Notice that $d \geq 0$ so that the particle on the interacting orbit is moving out *faster* than the corresponding free particle on the asymptote. At first sight, this seems surprising since the potential is attractive; the point is that because the potential is attractive, energy conservation implies that the interacting particle is moving faster than its asymptotic velocity.

The above suggests what we might expect in the quantum theory. In $\lim e^{iHt}e^{-iH_0t}$ we must expect to replace e^{-iH_0t} by $e^{-iH_0s(t)}$ where $s(t) = t + d \ln t$. Moreover, looking at the above, one sees that the constant d should be a function of the energy E, that is, e^{-iH_0t} should be replaced by $\exp[-iH_0 t - if(H_0) \ln t]$ for suitable f. To see what choice we should take for the modified quantum dynamics,

$$U_D(t) = \exp[-itH_0 - if(H_0) \ln t]$$

we note that in applying Cook's method to $\exp(it(H_0 + V))U_D(t)$, we shall have to estimate

$$\|[V - t^{-1}f(H_0)]U_D(t)\varphi\|$$

Now, since $U_D(t)$ is almost e^{-itH_0}, we expect, by Theorem IX.31 and also by stationary phase ideas that for large t, "x" will look like $2pt$ since $m = \frac{1}{2}$ if $H_0 = -\Delta$. Thus $x^{-1}U_D(t)\varphi$ will look like $\frac{1}{2}(pt)^{-1}U_D(t)\varphi$. Thus, to effect the cancellation we choose $f(H_0) = -\frac{1}{2}p^{-1}$, which is also the choice one would make on the basis of the classical solutions. To avoid a singularity at $t = 0$ and accommodate $H = -\Delta - \lambda r^{-1}$ we change things slightly and define

$$H_D(t) = H_0 - \tfrac{1}{2}\lambda(p|t|)^{-1}\theta(|4tH_0| - 1)$$

where $H_0 = -\Delta$ and $\theta(a)$ is the characteristic function of $(0, \infty)$. Let

$$U_D(t) = \exp\left(-i\int_0^t H_D(s)\, ds\right) \tag{156}$$

Notice that in (156) we can regard the integral as an integral of functions of p and then define $U_D(t)$ by the functional calculus as a multiplication operator in momentum space.

Theorem XI.71 Let $H_0 = -\Delta$, $H = -\Delta + V(r)$,

$$V(\mathbf{r}) = -\lambda r^{-1} + V_s(\mathbf{r}), \qquad \mathbf{r} \in \mathbb{R}^3$$

where $V_s(\mathbf{r})$ obeys (45). Then

$$\Omega_D^\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{iHt} U_D(t)$$

exist and define isometries with

$$e^{-iHs}\Omega_D^\pm = \Omega_D^\pm e^{-iH_0 s} \tag{157}$$

Proof We shall prove that

$$\|(H - H_D(t))U_D(t)\varphi\| \in L^1(\pm 1, \pm\infty) \tag{158}$$

for φ in a dense set $\mathscr{D}$ of L^2. From this estimate, the existence of $\Omega_D^\pm$ follows. The $\Omega_D^\pm$ are isometric since $U_D(t)$ is unitary. (157) follows as in the short-range case if one notes that (Problem 100)

$$\operatorname*{s-lim}_{t \to \pm\infty} U_D(t)^* U_D(t + s) = e^{-iH_0 s}$$

For $t > 0$, define

$$\tilde{H}_D(t) \equiv H_D(t) - H_0$$

and, for $t > 1/4p^2$,

$$A_D(t) \equiv \int_0^t \tilde{H}_D(s)\, ds = -\tfrac{1}{2}\lambda p^{-1}[\ln t + \ln(4p^2)]$$

(158) in the case $(1, \infty)$ follows from

$$\|V_s(r) \exp(-iH_0 t - iA_D(t))\varphi\| \in L^1(1, \infty) \tag{159a}$$

and

$$\|[-\lambda r^{-1} - \tilde{H}_D(t)] \exp(-iH_0 t - iA_D(t))\varphi\| \in L^1(1, \infty) \tag{159b}$$

(159a) holds for those φ with $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$ by an elementary modification (Problem 101) of the stationary phase method of Theorem XI.16. Let

$$\eta(x, t) = \exp(ix^2/4t) \exp(i\lambda t(2x)^{-1} \ln(x^2/t))$$

and for $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, define

$$R_\varphi(x, t) = U_D(t)\varphi(x) - (2it)^{-3/2}\eta(x, t)\hat{\varphi}(x/2t)$$

We shall show that R_φ satisfies

$$|R_\varphi(x, t)| \le C(\ln|t|)^\mu t^{-5/2}[1 + (x/t)^2]^{-m} \tag{160}$$

for all $|t| > 2$, any integer m, and suitable constants C and μ depending only on m and φ, and that (160) implies (159b).

We first note that (160) implies that

$$\lim_{t\to\infty} \|U_D(t)\varphi - (2it)^{-3/2}\eta(x, t)\hat{\varphi}(x/2t)\|_2 = 0 \tag{161}$$

for $\hat{\varphi} \in C_0^\infty$ and so for all φ. This is an analogue of (IX.33) and will be very relevant for the physical interpretation of $\Omega_D^\pm$ discussed below.

Let $\varphi_1 = (p^{-1}\hat{\varphi})^\vee$. Then for t sufficiently large

$$\begin{aligned}[(\lambda r^{-1} + \tilde{H}_D(t))U_D(t)\varphi](x) &= (\lambda x^{-1}U_D(t)\varphi)(x) - \lambda(2t)^{-1}(U_D(t)\varphi_1)(x)\\ &= \lambda x^{-1}R_\varphi(x, t) - \lambda(2t)^{-1}R_{\varphi_1}(x, t)\end{aligned}$$

since there is exact cancellation between the terms $\lambda x^{-1}\eta(x, t)\hat{\varphi}(x/2t)$ and $\lambda(2t)^{-1}\eta(x, t)\hat{\varphi}_1(x/2t)$. Now, by (160),

$$\|\lambda x^{-1}R_\varphi(x, t)\|^2 \le t^{-4}(\ln|t|)^{2\mu}$$

and similarly for the φ_1 term. Thus (159) follows if we can prove the estimate (160).

To prove (160), define $\varphi_C(x, t)$ by

$$\varphi_C(x, t) = [e^{-iA_D(t)}\varphi](x)$$

so that for t sufficiently large,

$$\hat{\varphi}_C(k, t) = \exp[\tfrac{1}{2}i\lambda k^{-1}\ln(4k^2t)]\hat{\varphi}(k)$$

Since $\hat{\varphi} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, we see that $\hat{\varphi}_C(\cdot, t) \in \mathscr{S}(\mathbb{R}^3)$, and for any norm $\|\cdot\|_\alpha$ on $\mathscr{S}$ and all t with $|t| > 2$,

$$\|\hat{\varphi}_C(\cdot, t)\|_\alpha \le C_\alpha \ln(|t|)^{\nu(\alpha)}$$

and thus

$$\|\varphi_C(\cdot, t)\|_\alpha \le D_\alpha \ln(|t|)^{\mu(\alpha)} \tag{162}$$

since $\hat{}$ is a homeomorphism of $\mathscr{S}$ to $\mathscr{S}$. Now we just follow the proof of Theorem IX.31: Using

$$(U_D(t)\varphi)(x) = (4\pi it)^{-3/2}\int e^{i(x-y)^2/4t}\varphi_C(y, t)\,dy$$

and

$$e^{i(x-y)^2/4t} = e^{ix^2/4t}e^{-ix\cdot y/2t}e^{iy^2/4t}$$

we see that

$$R_\varphi(x, t) = (4\pi it)^{-3/2}e^{ix^2/4t}\int e^{-ix\cdot y/2t}(e^{iy^2/4t} - 1)\varphi_C(y, t)\,dy \tag{163}$$

Using $|e^{iy^2/4t} - 1| \le |y^2/4t|$ and (162), we see that

$$|R_\varphi(x, t)| \le C|t|^{-5/2} \ln(|t|)^\mu$$

Similarly, from (163) and an integration by parts, we see that

$$\begin{aligned}\left|\left(\frac{x}{t}\right)^{2m} R_\varphi(x, t)\right| &\le |t|^{-3/2}\left|\int (-\Delta_y)^m[e^{-ix\cdot y/2t}](e^{iy^2/4t} - 1)\varphi_C(y, t)\, dy\right|\\ &\le |t|^{-3/2} \int |(-\Delta_y)^m[(e^{iy^2/4t} - 1)\varphi_C(y, t)]|\, dy\\ &\le C_m|t|^{-5/2}(\ln|t|)^{\mu(m)}\end{aligned}$$

so that

$$(1 + (x/t)^2)^{2m}|R_\varphi(x, t)| \le C_m|t|^{-5/2}(\ln|t|)^\mu$$

which proves (160). ▌

Before turning to the physical interpretation of $\Omega_D^\pm$, we note two consequences of their existence:

Corollary 1 Suppose that $V_s(\mathbf{r}) \to 0$ at ∞ as well as obeying (45). Then $\sigma_{\text{ac}}(H) = [0, \infty)$ where $H = -\Delta - \lambda|\mathbf{r}|^{-1} + V_s(r)$.

Corollary 2 If $\lambda \ne 0$ and H is given as above, the ordinary wave operators $\Omega^\pm(H, H_0)$ do not exist.

Corollary 1 is the standard consequence of (157). Corollary 2 is left to the reader (Problem 99).

We now turn to the physical interpretation of $\Omega_D^\pm$. Let $\psi = \Omega_D^+\varphi$ and define $\psi_t = e^{-iHt}\psi$, $\varphi_t^{(0)} = e^{-iH_0t}\varphi$, $\varphi_t^{(D)} = U_D(t)\varphi$. It is not true, as it would be in the short-range case, that $\|\varphi_t^{(0)} - \psi_t\| \to 0$ as $t \to -\infty$. Rather

$$\|\varphi_t^{(D)} - \psi_t\| \to 0 \qquad \text{as} \quad t \to -\infty$$

However, by (161) and (IX.33), we have that

$$\|\eta_t\varphi_t^{(0)} - \varphi_t^{(D)}\| \to 0 \qquad \text{as} \quad t \to \pm\infty$$

and

$$\|\gamma_t\hat{\varphi}_t^{(0)} - \hat{\varphi}_t^{(D)}\| = 0 \qquad \text{all } t$$

for suitable fixed functions $\eta_t(x)$ and $\gamma_t(k)$ of magnitude one. Thus, as $t \to -\infty$,.

$$\int \left| |\varphi_t^{(0)}(x)|^2 - |\psi_t(x)|^2 \right| dx \to 0$$

$$\int \left| |\hat{\varphi}_t^{(0)}(p)|^2 - |\hat{\psi}_t(p)|^2 \right| dp \to 0$$

Therefore, even though ψ_t is not an asymptotically free wave function, *its probability distributions* for both position and momentum approach those of the free wave function $\varphi_t^{(0)}$ as $t \to -\infty$. A similar statement holds as $t \to \infty$. In this sense the motion is "asymptotically free."

One can prove that $\Omega_D^\pm$ are complete if one makes stronger hypotheses:

Theorem XI.72 Suppose that

(i) V_s is $-\Delta$-bounded with relative bound $\alpha < 1$.
(ii) $V_s(H_0 + 1)^{-m-1}$ is trace class for some m.

Then $\Omega_D^\pm$ are complete in the sense that

$$\text{Ran } \Omega_D^+ = \text{Ran } \Omega_D^- = \mathscr{H}_{\text{ac}}(H)$$

This result can be proven by combining the reference in the Notes with Problem 102. We also remark that multichannel modified wave operators exist; see the Notes. Using the methods of Section 17, Enss has proven strong versions of this result. It seems likely that multichannel analogues will also be proven.

In the remainder of this section, we wish to discuss scattering theory for more general long-range potentials than Coulomb potentials. This general theory will illuminate the choice of $U_D(t)$.

Let us first consider the classical case. Suppose that $\mathbf{F} = -\nabla V$ with

$$\lim_{x \to \infty} V(\mathbf{x}) = 0 \tag{164a}$$

$$|\mathbf{F}(\mathbf{x})| \le k(1 + x)^{-1-\alpha} \tag{164b}$$

$$|\partial F_i(\mathbf{x})/\partial x_j| \le k(1 + x)^{-2-\alpha} \tag{164c}$$

where $\alpha > 0$. Of course, if $\alpha > 1$, we are in the short-range case of Section 2, so we suppose $\alpha < 1$. For convenience, we suppose that α^{-1} is not an integer.

We shall also suppose occasionally that F is "almost central" in the sense that for some $\varepsilon > 0$,

$$|\mathbf{F}_\perp(\mathbf{x})| \le k(1+x)^{-2-\varepsilon} \tag{165}$$

where $\mathbf{F}_\perp(\mathbf{x}) = \mathbf{F}(\mathbf{x}) - \mathbf{F}_\parallel(\mathbf{x})$ and $\mathbf{F}_\parallel(\mathbf{x}) = x^{-2}(\mathbf{x}\cdot\mathbf{F}(\mathbf{x}))\mathbf{x}$.

As in the short-range case, we consider

$$\dot{\mathbf{x}}(t) = \mathbf{p}(t), \qquad \dot{\mathbf{p}}(t) = -\nabla V, \qquad \mathbf{p}(0) = \mathbf{p}_0, \qquad \mathbf{x}(0) = \mathbf{x}_0 \tag{166}$$

and define

$$\Sigma_\pm = \left\{ \langle \mathbf{x}_0, \mathbf{p}_0 \rangle \in \mathbb{R}^6 \,\middle|\, V(\mathbf{x}_0) + \tfrac{1}{2}p_0^2 > 0 \text{ and the solution } \mathbf{x}(t) \text{ of (166) obeys } \overline{\lim_{t\to\mp\infty}}\, |\mathbf{x}(t)| = \infty \right\}$$

As in Section 2, one can show (Problem 103) that $\Sigma_+ = \Sigma_-$ almost everywhere and that for $\langle \mathbf{x}_0, \mathbf{p}_0\rangle \in \Sigma_\pm$ we have, for some $c > 0$,

$$|\mathbf{x}(t)| \ge c|t| - d \tag{167}$$

for all t with $\mp t \ge 0$.

Theorem XI.73 Let $\mathbf{F}$ and V obey (164).

(a) Let $\langle \mathbf{x}(t), \mathbf{p}(t)\rangle$ be a solution of (166) with initial data in Σ_+. Then

$$\lim_{t\to-\infty} \mathbf{p}(t) \equiv \mathbf{p}_{\text{in}}$$

exists. Moreover, $\mathbf{p}(t) - \mathbf{p}_{\text{in}} = O(|t|^{-\alpha})$ as $t \to -\infty$ and every value of $\mathbf{p}_{\text{in}} \ne 0$ occurs.

(b) If $\mathbf{x}_1(t)$, $\mathbf{x}_2(t)$ are two solutions with $\lim_{t\to-\infty} (\mathbf{p}_1(t) - \mathbf{p}_2(t)) = 0$, then

$$\mathbf{a} \equiv \lim_{t\to-\infty} (\mathbf{x}_1(t) - \mathbf{x}_2(t))$$

exists. Moreover, $|\mathbf{x}_1(t) - \mathbf{x}_2(t) - \mathbf{a}| = O(|t|^{-\alpha})$ as $t \to -\infty$, and for given $\mathbf{p}_{\text{in}} \ne 0$ and associated $\mathbf{x}_1$, every value of $\mathbf{a}$ occurs. If $\mathbf{a} = 0$, then $\mathbf{x}_2 = \mathbf{x}_1$ for all t; and if $\mathbf{a} = \mathbf{p}_{\text{in}} t_0$, then $\mathbf{x}_2(t) = \mathbf{x}_1(t - t_0)$.

(c) Suppose moreover that (165) holds. Then for any vector, $\mathbf{w}$ with $\mathbf{w} \cdot \mathbf{p}_{\text{in}} = 0$,

$$\lim_{t\to-\infty} \mathbf{x}(t)\cdot\mathbf{w} \equiv \alpha(\mathbf{w})$$

exists and $\mathbf{x}(t) \cdot \mathbf{w} - \alpha(\mathbf{w}) = O(|t|^{-\delta})$ where $\delta = \min\{\varepsilon, \alpha\}$. Every linear functional α on $\{\mathbf{w} | \mathbf{w} \cdot \mathbf{p}_{\text{in}} = 0\}$ occurs as one runs through all $\mathbf{x}$ with given $\mathbf{p}_{\text{in}} \neq 0$.

Proof Let $\langle x(t), p(t)\rangle$ be a solution with initial data in Σ_+. By (164b) and (167),

$$|F(x(t))| \leq k(1 + |x(t)|)^{-1-\alpha} \leq C_1(1 + |t|)^{-1-\alpha}$$

so that

$$\lim_{t\to-\infty} p(t) = p_0 + \lim_{t\to-\infty} \int_0^t F(x(s))\, ds$$

exists and we have $p(t) - p_{\text{in}} = O(|t|^{-\alpha})$. We defer the proof that every value of $p_{\text{in}} \neq 0$ occurs.

Let x_1, x_2 be two solutions with the same value of p_{in}. Let $\Delta(t) = x_1(t) - x_2(t)$. Then

$$|\dot{\Delta}(t)| = |p_1(t) - p_2(t)| \leq \int_{-\infty}^t |F(x_1(s)) - F(x_2(s))|\, ds$$

since $p_i(t) = p_{\text{in}} + \int_{-\infty}^t F(x_i(s))\, ds$. Now, by (164c) and (167),

$$|F(x_1(t) - F(x_2(t))| \leq C_2 |\Delta(t)|(1 + |t|)^{-2-\alpha}$$

so that

$$|\dot{\Delta}(t)| \leq \int_{-\infty}^t |\Delta(s)|(1 + |s|)^{-2-\alpha}\, ds \tag{168}$$

Now suppose that $|\Delta(t)| \leq C_\gamma |t|^\gamma$, $\alpha < \gamma \leq 1$ for $t \leq -1$. Then by (168), $|\dot{\Delta}(t)| \leq C(1 + \alpha - \gamma)^{-1}|t|^{-1-\alpha+\gamma}$ so that

$$|\Delta(t)| = \left|\Delta(-1) + \int_{-1}^t \dot{\Delta}(s)\, ds\right| \leq C'_\gamma |t|^{\gamma-\alpha}$$

Note that $|\Delta(t)| \leq C|t|$. So, using the above N times, where N is chosen so that $\alpha N < 1$, $\alpha(N + 1) > 1$, we have that $|\Delta(t)| \leq C'|t|^{1-N\alpha}$. Then, by (168), for $t < 0$,

$$|\dot{\Delta}(t)| \leq C((N + 1)\alpha)^{-1}|t|^{-(N+1)\alpha}$$

so that $\lim_{t\to-\infty} \Delta(t) = \Delta(0) + \lim_{t\to-\infty} \int_0^t \dot{\Delta}(s)\, ds$ exists. This means that $\Delta(t)$ is bounded, and thus by (168), $\Delta(t) - a = O(|t|^{-\alpha})$. Again we defer the proof that every a occurs.

If $a = 0$, then $\Delta(t) \to 0$ as $t \to -\infty$. As a result, by (168), we can write for $t < 0$

$$|\Delta(t)| \leq (2 + \alpha)^{-1}(1 + \alpha)^{-1}(1 + |t|)^{-\alpha} \sup_{-\infty \leq s < t} |\Delta(s)|$$

Choosing t so that $(2+\alpha)^{-1}(1+\alpha)^{-1}(1+|t|)^{-\alpha} < 1$, we conclude that $\Delta(s) = 0$ for $s \le t$ so that $\Delta(t) = 0$ for all t by local uniqueness.

Given t_0 and $x_1(t)$, it is easily seen that $x_3(t) \equiv x_1(t - t_0)$ obeys $\dot{x}_3(t) \to p_{\text{in}}$ and $x_1(t) - x_3(t) = \int_{t-t_0}^{t} \dot{x}_1(s)\, ds \to p_{\text{in}} t_0$. By the uniqueness just proven, any x_2 with $\dot{x}_2 \to p_{\text{in}}$ and $x_1 - x_2 \to p_{\text{in}} t_0$ is equal to x_3.

Now suppose that (165) holds and let $w \cdot p_{\text{in}} = 0$. Suppose that $|w \cdot F(x(t))| \le C|t|^{-\gamma}$ where $1 < \gamma < 2$. Then, since

$$w \cdot p(t) = \int_{-\infty}^{t} w \cdot F(x(s))\, ds \tag{169}$$

$$w \cdot x(t) = w \cdot x(0) + \int_0^t (p(s) \cdot w)\, ds$$

we have

$$|w \cdot x(t)| \le C_2(1 + |t|)^{2-\gamma}$$

So, by (167),

$$|w \cdot x(t)|\, |x(t)|^{-1} \le C_4(1 + |t|)^{1-\gamma}$$

As a result, using

$$|a \cdot F(x(s))| \le |F_\perp(x(s))|\, |a| + \frac{|a \cdot x(s)|}{|x(s)|}\, |F(x(s))|$$

we have by (164b) and (165),

$$|w \cdot F(x(t))| \le (\text{const})[(1 + |t|)^{-2-\varepsilon} + (1 + |t|)^{-\gamma-\alpha}]$$

By repeating this process, beginning with $\gamma = 1 + \alpha$,

$$|w \cdot F(x(t))| \le (\text{const})(1 + |t|)^{-2-\delta}$$

where $\delta = \min(\varepsilon, \alpha)$. Thus, using (169), we have that $w \cdot p(t) = O(|t|^{-1-\delta})$, so $w \cdot x(t)$ has a limit $\alpha(w)$ and $w \cdot x(t) - \alpha(w) = O(|t|^{-\delta})$.

Finally, we return to the question of existence, that is, that every $\mathbf{p}_{\text{in}} \ne 0$ and $\mathbf{a}$ occurs; this will automatically imply that every α occurs for the linear map $w \mapsto \alpha(w)$. Obviously, it suffices to construct an auxiliary function $\mathbf{z}(\mathbf{p}, t)$ so that $\lim_{t\to-\infty} \dot{\mathbf{z}}(\mathbf{p}, t) = \mathbf{p}$ and then for any $\mathbf{a}$, a solution $\mathbf{x}(t)$ with $\lim_{t\to-\infty} (\mathbf{x}(t) - \mathbf{z}(\mathbf{p}, t)) = \mathbf{a}$ and $\lim_{t\to-\infty} \dot{\mathbf{x}}(t) = \mathbf{p}$. $\mathbf{z}$ will replace the elementary $\mathbf{p}t$ used in the short-range case. Once, we have the "right" $\mathbf{z}(\mathbf{p}, t)$, we shall construct the solution $\mathbf{x}$ by the contraction mapping theorem as in the short-range case.

How can one find a good choice for $\mathbf{z}(\mathbf{p}, t)$? To get an approximate value of $\dot{\mathbf{z}}$ which will go to $\mathbf{p}$ as $t \to -\infty$, we shall try to integrate from $t = -\infty$.

However, we shall not be able to get $\mathbf{z}$ by integrating $\dot{\mathbf{z}}$ from $-\infty$ since $\dot{\mathbf{z}}$ will approach $\mathbf{p}$ only as a power $|t|^{-\alpha}$ with $\alpha < 1$. Thus we shall integrate $\dot{\mathbf{z}}$ from $t = 0$. Therefore we define $\mathbf{z}_n(\mathbf{p}, t)$ inductively by

$$\mathbf{z}_0(\mathbf{p}, t) = \mathbf{p}t$$

$$\dot{\mathbf{z}}_n(\mathbf{p}, t) = \mathbf{p} + \int_{-\infty}^{t} \mathbf{F}(\mathbf{z}_{n-1}(\mathbf{p}, s))\, ds$$

$$\mathbf{z}_n(\mathbf{p}, t) = \int_0^t \dot{\mathbf{z}}_n(\mathbf{p}, s)\, ds$$

We take $z(p, t) = z_N(p, t)$ where $N = [1/\alpha]$, the integral part of $1/\alpha$. Clearly, for any fixed $p \neq 0$ and $t \leq 0$,

$$|z_n(p, t)| \geq c|t| - d \tag{170}$$

for $n = 0, \ldots, N$ and some $c > 0$. Moreover, by a simple inductive argument of the type we have already used,

$$|z_n(p, t) - z_{n-1}(p, t)| \leq Kt^{1-n\alpha} \tag{171}$$

for $n = 1, \ldots, N$. Now, if x obeys

$$\ddot{x}(t) = F(x(t))$$

$$x(t) - z_N(p, t) - a \to 0$$

$$\dot{x}(t) - \dot{z}_N(p, t) \to 0$$

then $y(t) = x(t) - z_N(p, t) - a$ obeys

$$y(t) = \int_{-\infty}^{t} \int_{-\infty}^{w} [F(z_N(p, s) + a + y(s)) - F(z_{N-1}(p, s))]\, ds\, dw \tag{172}$$

Conversely, solutions of (172) yield solutions of Newton's equation with the desired asymptotic behavior. Given (164c), (170), and (171), one can mimic the contraction mapping method of Section 2 (Problem 104) and find solutions of (172) and to obtain the existence result needed to complete the proof. ▮

What is the physical interpretation of this theorem? Consider the case where both (164) and (165) hold. Then, given $\mathbf{p}_{\text{in}} \neq 0$ and $\mathbf{b}_{\text{in}}$ perpendicular to $\mathbf{p}_{\text{in}}$, there is a one-parameter family of solutions x_s with

$$\dot{\mathbf{x}}_s(t) \to \mathbf{p}_{\text{in}}$$

$$\mathbf{x}_s(t) - \mathbf{p}_{\text{in}}(\mathbf{p}_{\text{in}} \cdot \mathbf{x}(s))p_{\text{in}}^{-2} \to \mathbf{b}_{\text{in}}$$

as $t \to -\infty$. They differ only by time parameterization, that is, $x_s(t) = x_0(t-s)$. Thus, if $\langle \mathbf{x}_s(0), \dot{\mathbf{x}}_s(0) \rangle \in \Sigma_-$ (and this will happen for almost all $\mathbf{p}_{\text{in}}$, $\mathbf{b}_{\text{in}}$; see Problem 105), $\lim_{t\to\infty} \dot{\mathbf{x}}_s(t) \equiv \mathbf{p}_{\text{out}}$ and

$$\lim_{t\to\infty} [\mathbf{x}_s(t) - \mathbf{p}_{\text{out}}(\mathbf{p}_{\text{out}} \cdot \mathbf{x}(s))p_{\text{out}}^{-2}] \equiv \mathbf{b}_{\text{out}}$$

are independent of s. As a result, one has a natural definition of a map

$$\tilde{S}\colon \langle \mathbf{p}_{\text{in}}, \mathbf{b}_{\text{in}} \rangle \to \langle \mathbf{p}_{\text{out}}, \mathbf{b}_{\text{out}} \rangle$$

As in the short-range case, if the force is central, $\mathbf{b}_{\text{out}}$ is completely determined by $\mathbf{p}_{\text{out}}$ and conservation of angular momentum, so that S is described by giving a single scattering angle as a function of $\mathbf{p}_{\text{in}}$ and $\mathbf{b}_{\text{in}}$. The point is that we can see precisely what is lost in going from short-range to long-range; namely in the long-range case, there is no finite time delay. In fact, one can show (Problem 106) that if $V_\varepsilon(x)$ is some short-range modification of V, say $V_\varepsilon(x) = e^{-\varepsilon x^2} V(x)$, then as $\varepsilon \to 0$ the part of the scattering operator given by $\tilde{S}_\varepsilon$ converges to the $\tilde{S}$ defined above. Typically the time delays will diverge as $\varepsilon \to 0$ if V is truely long-range.

The above discussion suggests that the problem of long-range quantum scattering should be connected with infinite, energy-dependent phases since classical time delay is analogous to the phase of the quantum scattering operator. The changes from the ordinary to the modified dynamics can be viewed precisely as an infinite energy dependent adjustment of phase. Unfortunately, the above formulation does not have a quantum generalization because the map $\langle p, a \rangle \to z_N(p, t) + a$ for fixed t is *not* in general a canonical transformation, so that it will not in general correspond in quantum mechanics to a unitary operator. One can sometimes construct approximate solutions $\tilde{z}(p, a, t)$ so that $\langle p, a \rangle \to \tilde{z}(p, a, t)$ is a canonical transformation for each t and so that there is a solution $x(p, a, t)$ of (166) with $|x - \tilde{z}| + |\dot{x} - \dot{\tilde{z}}| \to 0$ as $t \to -\infty$ and $\dot{\tilde{z}}(p, a, t) \to p$, $\tilde{z}(p, a, t) - \tilde{z}(p, b, t) \to a - b$ as $t \to -\infty$. It is the analogue of this classical construction that we shall follow in the quantum case below. One can reprove Theorem XI.73 by following the arguments that we shall give in the quantum case below in the classical case, and thereby one can obtain a proof with an approximate dynamics which *is* given by a canonical transformation; see the reference in the Notes and Problem 107.

Theorem XI.74 Let $V = V_L + V_s$ be a measurable function on $\mathbb{R}^n$ so that V_s obeys (45) and V_L obeys

$$|(D^\alpha V_L)(x)| \le C(1 + x)^{-|\alpha| - \varepsilon}; \qquad |\alpha| \le M$$

where $\varepsilon > \frac{1}{2}$ if $M = 1$, $\varepsilon > \frac{1}{3}$ if $M = 2$, and $\varepsilon > 0$ if $M = 3$. Then, there exists a C^∞ function $W(\mathbf{k}, t)$ for $\mathbf{k} \in \mathbb{R}^n \backslash \{0\}$, $t \in \mathbb{R}$, so that

(a) $W(k, s + t) - W(k, t) \to \frac{1}{2}sk^2$ (173)
as $t \to \pm\infty$ for each fixed k, s.

(b) For any self-adjoint extension H of $-\frac{1}{2}\Delta + V$ on $C_0^\infty(\mathbb{R}^n)$,

$$\operatorname*{s-lim}_{t \to \mp\infty} e^{iHt} U_D(t) \equiv \Omega_D^\pm$$

exist where $U_D(t) = \exp(-iW(-i\nabla, t))$.

The full proof of this result involves many detailed estimates. We shall not give it here, but will describe several important aspects including the method for constructing W.

The point of (173) is that it implies (Problem 100) that

$$\operatorname*{s-lim}_{t \to \pm\infty} [U_D(t + s) U_D(t)^{-1}] = e^{-isH_0}$$

so that the usual intertwining relation holds:

$$e^{-isH} \Omega_D^\pm = \Omega_D^\pm e^{-isH_0}$$

Of course, one can object that W may not be uniquely determined, and in fact it is not. However, if W and W' are two functions for which (a) and (b) hold and if $\operatorname{Ran} \Omega_D^+ = \mathscr{H}_{\text{ac}}(H)$, then (Problem 108) there is a measurable function $F(k)$ that is finite a.e. so that

$$(\Omega_D^+)' = \Omega_D^+ e^{iF(-i\nabla)}$$

In particular, $\operatorname{Ran} \Omega_D^+$ is independent of W and so asymptotic completeness holds for one choice of W if and only if it holds for any other choice.

In addition, one can show that for any choice of W, the asymptotic *probability distribution* of $U_D(t)f$ in both x and p space is the same as that of $e^{-itH_0}f$. Of course, if $(\Omega_D^\pm)' = \Omega_D^\pm e^{iF_\pm(k)}$, then the kernel of the on-energy-shell S-operators obeys

$$S'(k, k') = S(k, k') e^{i(F_+(k) - F_-(k'))}$$

so that the differential cross sections will also be independent of the choice of W. Unfortunately the "phase" of $S(k, k')$ is not determined until one makes a choice of W. The question of what is the "right phase" is an interesting question which we discuss in the notes.

We now turn to three aspects of the proof of Theorem XI.74: (i) smoothing V_L, (ii) choosing W, (iii) some remarks on the detailed estimates.

Clearly, given V obeying the hypothesis of Theorem XI.74, there will be many decompositions of V into $V_L + V_s$ where V_s obeys (45). The first step is to pick a decomposition such that V_L is C^∞ with derivatives that fall off more and more rapidly at infinity. In fact one can construct such a decomposition with

$$|(D^\alpha V_L)(x)| \leq C_\alpha(1+x)^{-m(|\alpha|)} \tag{174a}$$

for all α where

$$m(1) + m(3) > 4 \tag{174b}$$

and

$$m(\ell) \geq \delta\ell - \varepsilon \tag{174c}$$

$\delta > \frac{1}{2}$. For example (Problem 109), in the case $\varepsilon > 0$, $M = 3$, one can take $m(1) = 1 + \varepsilon$, $m(2) = 2 + \varepsilon$, $m(3) = 3 + \varepsilon$, $m(\ell) = 3 + \varepsilon + \frac{2}{3}(\ell - 3)$ for $\ell > 3$. How does one construct V_L? Begin with a breakup $\tilde{V}_s + \tilde{V}_L = V$. The obvious first guess for V_L would be $f = h * \tilde{V}_L$ where h is in C_0^∞. f is C^∞, but higher derivatives will not automatically fall off since $\tilde{V}_L$ may only be C^1 and $D^\alpha h$ has no "falloff." Somehow even though h is fixed, one wants it to be more and more spread out as $x \to \infty$! To arrange this, one writes $\tilde{V}_L = \sum \tilde{V}_L^{(n)}$ where $\tilde{V}_L^{(n)}$ have support in wider and wider spherical shells which march out to infinity. Then we take $V_L = \sum h_n * \tilde{V}_L^{(n)}$ where the h_n become more and more spread out. To get $V_L - \tilde{V}_L$ short-range, one needs an additional trick. The construction for the case $\varepsilon > 0$, $M = 3$ is outlined in Problem 109.

As we shall explain later, (174b) is critical. It clearly holds in case $M = 3$, $\varepsilon > 0$; and it is the reason that for $\varepsilon > 0$, $M = 3$ always works and we never need a priori information on $D^\alpha V_L$ with $|\alpha| \geq 4$. It also is the reason one needs $\varepsilon > \frac{1}{2}$ (respectively, $\varepsilon > \frac{1}{3}$) if $M = 1$ (respectively, 2). When one goes through the above construction of a new V_L, these values of ε are required to assure (174b) (see Problem 110).

Next, we turn to the construction of W. In applying Cook's method to control the limit $\Omega_D^\pm$ one has to estimate

$$\iint\left(\frac{1}{2}k^2 + V(x) - \frac{\partial W}{\partial t}\right)e^{ik\cdot x - iW(k,t)}\hat{\varphi}(k)\,dx\,dk$$

The short-range piece of V should be controlled as in the short-range case. The long-range case will have to be cancelled in part by $\partial W/\partial t$ as in the Coulomb case. If the method of stationary phase is used, we expect that the above integral will be concentrated near points where $x = \partial W/\partial k$. Thus, to effect as great a cancellation as possible, one might try to solve

$$V_L\left(\frac{\partial W}{\partial k}\right) + \frac{k^2}{2} = \frac{\partial W}{\partial t} \tag{175}$$

Before discussing exact solutions of this nonlinear partial differential equation, we want to write it in some alternative forms and discuss approximate solutions. It is natural to think of $U_D(t)$ as coming from integrating a time dependent equation with Hamiltonian

$$H(t) = H_0 + f(-i\nabla, t)$$

Clearly, we should choose

$$f(k, t) \equiv \frac{\partial W}{\partial t} - \frac{k^2}{2} \tag{176}$$

If we define $x(k, t) \equiv \partial W/\partial k$, then (175) becomes

$$f(k, t) = V_L(x(k, t)) \tag{177}$$

Now by applying $\partial/\partial k$ to (175), one sees that $x(k, t)$ obeys the differential equation

$$\dot{x}(k, t) = k + \nabla_k V_L(x(k, s)) \tag{178}$$

If we try to choose $W \equiv 0$ for $t = t_0$, then (177) and (178) give the integral equation

$$f(k, t) = V_L\left(kt - kt_0 + \int_{t_0}^{t} \nabla_k f(k, s)\, ds\right) \tag{179}$$

The simplest approximate solution of (179) is to take $t_0 = 0$ and

$$f(k, t) \approx V_L(kt)$$

Using

$$W(k, t) = \tfrac{1}{2}k^2 t + \int_{t_0}^{t} f(k, s)\, ds + \text{const}$$

we see that this approximation leads to the choice of W we used in the Coulomb case. This choice can be used to define modified wave operators for $V_L(x) = |x|^{-\alpha}$, so long as $\alpha > \frac{1}{2}$. For $\alpha < \frac{1}{2}$, it is necessary to try either to solve (175) exactly or go to a higher approximation of (179), for example,

$$f(k, t) \approx V_L\left(kt + \int_0^t s(\nabla V_L)(ks)\, ds\right)$$

This method of higher approximation has been used, but it turns out to require information about more and more derivatives of V_L as $\alpha \to 0$.

The key to the proof of Theorem XI.74 is the construction of *exact* solutions of (175) which result from realizing that it is a standard equation of the advanced theory of classical mechanics, namely the momentum space **Hamilton–Jacobi equation.** We can now give a formal construction of solutions of (175). Let $g(\eta)$ be an arbitrary smooth function on $\mathbb{R}^n$ (or a subset of $\mathbb{R}^n$). Fix t_0 real. Let $X(\eta, t)$ be the solution of Newton's equation

$$\ddot{X}(\eta, t) = -(\nabla V_L)(X(\eta, t))$$

with initial conditions

$$X(\eta, t_0) = g(\eta) \tag{180a}$$

$$\dot{X}(\eta, t_0) = \eta \tag{180b}$$

Suppose that for each fixed t, the map $\eta \mapsto k \equiv \dot{X}(\eta, t)$ is invertible, with inverse function $\eta = N(k, t)$, that is,

$$\dot{X}(N(k, t), t) = k \tag{181}$$

Define

$$x(k, t) = X(N(k, t), t) \tag{182}$$

that is, x is the position at time t of that solution of Newton's equation obeying (180) which has velocity k at time t. We claim that x obeys (178) so that we can recover solutions of (179) by using (176) and (177). To check that x obeys (178), we first differentiate (181) with respect to k and t to obtain

$$\frac{\partial \dot{X}}{\partial \eta} \frac{\partial N}{\partial k} = 1 \tag{183}$$

$$\frac{\partial \dot{X}}{\partial \eta} \frac{\partial N}{\partial t} + \frac{\partial \dot{X}}{\partial t} = 0$$

so that, using $\ddot{X}(\eta, t) = -(\nabla V_L)(X)$, we obtain

$$\frac{\partial \dot{X}}{\partial \eta} \frac{\partial N}{\partial t} = (\nabla V_L)(x) \tag{184}$$

From (182), we obtain

$$\frac{\partial x}{\partial k} = \frac{\partial X}{\partial \eta} \frac{\partial N}{\partial k} \tag{185}$$

From (183)–(185), we see that

$$\frac{\partial N}{\partial t}\frac{\partial X}{\partial \eta} = (\nabla V_L)(x)\frac{\partial x}{\partial k} = \frac{\partial}{\partial k} V_L(x(k, t))$$

so that

$$\begin{aligned} \dot{x}(k, t) &= \frac{\partial X}{\partial t} + \frac{\partial X}{\partial \eta}\frac{\partial N}{\partial t} \\ &= k + \frac{\partial}{\partial k} V_L(x(k, t)) \end{aligned}$$

which is (178).

The only "formal" aspect of the above involves the invertibility of $\eta \mapsto \dot{X}(\eta, t)$. By using the asymptotic information on V_L, one can construct a function $W(k, t)$ on $\{\mathbb{R}^n\backslash\{0\}\} \times \mathbb{R}$ such that for any compact $K \subset \mathbb{R}^n\backslash\{0\}$, there is a T_K with W obeying (175) on $K \times \{t \mid |t| > T_K\}$. This is the function W used to construct the generalized wave operators.

Finally, we turn to some aspects of the estimates. The importance of (174b) comes from the fact that when it holds, one can show that W obeys

$$|D_k^\alpha(t^{-1}\, \partial W/\partial k - k)| \le Ct^{-\beta}, \qquad |\alpha| \le 1$$

for some $\beta > 0$. This means that for t large the critical points of $x \cdot k - W(k, t)$ that are solutions of

$$x/t = k + t^{-1}(\partial W/\partial k - tk)$$

are unique and are near the short-range critical point $x/t = k$. The other aspect of the detailed estimates that we should mention is that one must push stationary phase methods even further than we do in Theorem XI.15. After rewriting

$$\int u(k)e^{i\omega f(k)}\, dk = \int v(y)e^{i\omega(y,\, Ay)/2}\, dy$$

as we do there and using (43), one must make an expansion of $e^{i(k,\, A^{-1}k)/2\omega}$ in powers of ω^{-1} rather than using the simple estimate used in Theorem XI.15.

XI.10 Optical and acoustical scattering I: Schrödinger operator methods

In this section we present techniques for describing the scattering of classical waves in inhomogeneous media. The methods are geared to linear wave equations and are applicable to acoustic and optical scattering. The basic physical situation is as follows. Suppose that we have an inhomogeneous medium that looks more and more homogeneous as $x \to \infty$. The propagation of acoustical or optical waves in the medium will be governed by a linear wave equation with nonconstant coefficients because of the inhomogeneity. If the initial disturbance is of finite energy, then as t gets large the waves should propagate out toward infinity. As they do so, they should look more and more like solutions of the corresponding equations with constant coefficients. Thus, we should be able to develop a scattering theory that relates the solutions of the nonconstant coefficient equation to the solutions of the corresponding equation with constant coefficients.

The basic idea in this section is to formulate both the homogeneous and inhomogeneous equations as Hilbert space problems so that we can use the methods developed earlier in this chapter. This will lead us necessarily to the problem of comparing unitary groups on two *different* Hilbert spaces. In the next section we describe another approach to these problems due to Lax and Phillips. To see how the problem of two Hilbert spaces arises, we begin with an example.

Example 1 (acoustical scattering in inhomogeneous media) The propagation of sound waves in a homogeneous medium can be described by specifying at each time t the function $u(x, t)$ which is the difference between the pressure at x and the equilibrium pressure. If one linearizes the nonlinear equations of fluid dynamics about the equilibrium pressure, an approximation that is good for small u, one obtains the wave equation

$$\begin{aligned} u_{tt}(x, t) &= c_0^2\, \Delta u(x, t) \\ u(x, 0) = f(x), &\qquad u_t(x, 0) = g(x) \end{aligned} \tag{186}$$

where f and g are specified by the initial disturbance and c_0 is the velocity of propagation of the pressure waves.

Now, if the medium in which the waves are traveling has a density $\rho(x)$ that varies with position, then the pressure will satisfy the more complicated equation

$$\begin{aligned} u_{tt}(x, t) &= c(x)^2 \rho(x) \nabla \cdot \frac{1}{\rho(x)} \nabla u \\ u(x, 0) = f(x), &\qquad u_t(x, 0) = g(x) \end{aligned} \tag{187}$$

where the velocity $c(x)$ will also vary with position since the density does. Suppose that

$$c(x) \to c_0, \qquad \rho(x) \to \rho_0 \tag{188}$$

as $|x| \to \infty$. If this convergence is rapid enough, then we should be able to develop a scattering theory for (186) and (187) since we expect the solutions of (187) to propagate out toward ∞. And, when they are out near infinity, they should look very much like solutions of (186).

We formulate both equations as Hilbert space problems using the ideas in Section X.13. We deal with (186) first. Let $H_0 = -c_0^2 \Delta$ on $L^2(\mathbb{R}^3)$ and $B_0 = \sqrt{H_0}$. Denote by $[D(B_0)]$ the closure of $D(B_0)$ in the norm $\|B_0 u\|_2$. Note that $[D(B_0)]$ contains ideal elements that are not in $L^2(\mathbb{R}^3)$ because zero is in $\sigma(B_0)$. Let $\mathscr{H}_0$ be the Hilbert space

$$\mathscr{H}_0 = [D(B_0)] \oplus L^2(\mathbb{R}^3)$$

with norm

$$\|\langle u, v\rangle\|^2 = \|B_0 u\|_2^2 + \|v\|_2^2$$

and define

$$A_0 = i\begin{pmatrix} 0 & I \\ -B_0^2 & 0 \end{pmatrix}, \qquad D(A_0) = D(B_0^2) \oplus D(B_0)$$

where

$$D(B_0^2) = \{u \in [D(B_0)] \mid B_0 u \in D(B_0)\}$$

and we are denoting both B_0 and its extension to $[D(B_0)]$ by B_0. Then A_0 is self-adjoint on $D(A_0)$ and (186) may be reformulated as

$$\begin{aligned} \varphi'(t) &= -iA_0 \varphi(t) \\ \varphi(0) &= \varphi_0 \equiv \langle f, g\rangle \end{aligned} \tag{189}$$

for the $\mathscr{H}_0$-valued function $\varphi(t) = \langle u(t), u_t(t)\rangle$. The solution is given by $\varphi(t) = W_0(t)\varphi_0$ where

$$W_0(t) = e^{-iA_0 t} = \begin{pmatrix} \cos B_0 t & B_0^{-1} \sin B_0 t \\ -B_0 \sin B_0 t & \cos B_0 t \end{pmatrix}$$

with the matrix entries defined by the functional calculus. If $\varphi_0 \in D(A_0)$, then $\varphi(t)$ is strongly differentiable and satisfies (189), which implies that the first component $u(t)$ satisfies (186). It will later be convenient to change the inner product on $L^2(\mathbb{R}^3)$ by a fixed constant.

In order to deal with (187), we assume in addition to (188) that

$$0 < \rho_1 \le \rho(x) \le \rho_2 < \infty \qquad \text{for all } x \tag{190a}$$

$$0 < c_1 \le c(x) \le c_2 < \infty \qquad \text{for all } x \tag{190b}$$

If in addition ρ is C^1, then

$$H_1 = -c(x)^2\rho(x)\nabla \cdot \rho(x)^{-1}\nabla$$

is a well-defined operator on $C_0^\infty(\mathbb{R}^3)$. But it is clear that it is not even formally symmetric in the usual L^2 inner product because of the factor $c(x)^2\rho(x)$. However, if we define $L^2_{\rho c}(\mathbb{R}^3)$ to be $L^2(\mathbb{R}^3)$ with the inner product

$$(f, g)_{\rho c} = (f, (c^2\rho)^{-1}g)_{L^2(\mathbb{R}^3)}$$

then in this new inner product H_1 is obviously symmetric on $C_0^\infty(\mathbb{R}^3)$. Notice that, by (190a), $L^2_{\rho c}$ and L^2 are equal as sets; in fact, the norms are equivalent. Associated to H_1 on $C_0^\infty(\mathbb{R}^3) \subset L^2_{\rho c}$ is the quadratic form

$$\begin{aligned} q_1(f, g) = (f, H_1 g)_{\rho c} &= (f, -\nabla \cdot \rho^{-1}\, \nabla g)_{L^2} \\ &= (\nabla f, \rho^{-1}\, \nabla g)_{L^2} \end{aligned}$$

The form q_1 is positive and closable by assumption (190a). In fact, since

$$\rho_2^{-1}(\nabla f, \nabla f)_2 \le (\nabla f, \rho^{-1}\, \nabla f)_2 \le \rho_1^{-1}(\nabla f, \nabla f) \tag{191}$$

the closure of q_1 has form domain $Q(-\Delta)$. Let H_1 be the self-adjoint operator on $L^2_{\rho c}$ corresponding to the closure of q_1 according to Theorem VIII.15. We now proceed as before by defining $B_1 = \sqrt{H_1}$, $[D(B_1)]$ to be the closure of $D(B_1)$ in the norm $\|B_1 u\|_{\rho c}$, and

$$\mathscr{H}_1 = [D(B_1)] \oplus L^2_{\rho c}(\mathbb{R}^3)$$

$$A_1 = i\begin{pmatrix} 0 & I \\ -B_1^2 & 0 \end{pmatrix}$$

Then A_1 is self-adjoint on $D(B_1^2) \oplus D(B_1)$ and generates

$$W_1(t) = \begin{pmatrix} \cos B_1 t & B_1^{-1} \sin B_1 t \\ -B_1 \sin B_1 t & \cos B_1 t \end{pmatrix}$$

As before, if $\varphi_0 \in D(A_1)$, then $u(t)$, the first component of

$$\varphi(t) = W_1(t)\varphi_0$$

satisfies (187). Notice that the above construction of H_1 did not require any regularity on $c(x)$ or $\rho(x)$. However, if they are both smooth, then H_0 and H_1 are both essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ (see Problem 66).

In order to develop a scattering theory for (187), we must compare $W_1(t)$ on $\mathscr{H}_1$ to $W_0(t)$ on $\mathscr{H}_0$. The domains of B_0 and B_1 are both equal to $Q(-\Delta)$; and, by (191), we have

$$\rho_2^{-1}\|B_0 u\|_2^2 \le \|B_1 u\|_{\rho c}^2 \le \rho_1^{-1}\|B_0 u\|_2^2 \tag{192}$$

so $\mathscr{H}_0$ and $\mathscr{H}_1$ are equal as sets, but they have different (though equivalent) inner products. If we restrict ourselves to one inner product, then one of the two groups will not be unitary. We are thus in a situation where it is natural to apply the two Hilbert space formalism outlined in Section 3.

In order to study the kind of situation described in the above example, we formulate the problem abstractly. Let H_0 and H_1 be nonnegative self-adjoint operators on Hilbert spaces $\mathscr{K}_0$ and $\mathscr{K}_1$. To make the presentation easier we shall assume that H_0 and H_1 have no point spectrum at zero; the general case is treated in the references given in the Notes. We want to develop a scattering theory for the two equations

$$u_0''(t) = -H_0 u_0(t)$$
$$u_1''(t) = -H_1 u_1(t)$$

when we are given a "natural" unitary identification operator $V: \mathscr{K}_0 \to \mathscr{K}_1$. Let $\mathscr{H}_0$ and $\mathscr{H}_1$ be the Hilbert spaces

$$\mathscr{H}_0 = [D(B_0)] \oplus \mathscr{K}_0$$
$$\mathscr{H}_1 = [D(B_1)] \oplus \mathscr{K}_1$$

constructed as in the example with $B_k = \sqrt{H_k}$ and with norms

$$\|\langle u, v\rangle\|_0^2 = \|B_0 u\|_{\mathscr{K}_0}^2 + \|v\|_{\mathscr{K}_0}^2$$
$$\|\langle u, v\rangle\|_1^2 = \|B_1 u\|_{\mathscr{K}_1}^2 + \|v\|_{\mathscr{K}_1}^2$$

The solutions of the above equations are given by

$$\begin{pmatrix} u_k(t) \\ u_k'(t) \end{pmatrix} = W_k(t) \begin{pmatrix} u_k(0) \\ u_k'(0) \end{pmatrix}$$

where

$$W_k(t) = \begin{pmatrix} \cos B_k t & B_k^{-1} \sin B_k t \\ -B_k \sin B_k t & \cos B_k t \end{pmatrix}$$

As in the example, we denote the generator of $W_k(t)$ by A_k.

Our plan of attack is to reduce the questions of existence and completeness of the wave operators for $W_0(t)$, $W_1(t)$ to the same questions for $V^{-1} H_1 V$ and H_0 on $\mathscr{K}_0$. In this way the two Hilbert space problem is reduced to a single Hilbert space problem involving operators similar to the Schrödinger operators which we have already studied. We shall later show how one can stay in the two Hilbert space setting and apply Theorem XI.13 (see Example 1, revisited). We use without comment the notation and terminology of two Hilbert space scattering introduced in Section 3.

We begin by choosing an identification operator J between $\mathscr{H}_0$ and $\mathscr{H}_1$ which is mathematically convenient but physically unnatural. Later we shall show that under certain circumstances, usually fulfilled in applications, other more natural identification operators are (asymptotically A_0-) equivalent to J. We define $J: \mathscr{H}_0 \to \mathscr{H}_1$ by

$$J: \langle u, v \rangle \mapsto \langle B_1^{-1} V B_0 u, Vu \rangle$$

Theorem XI.75 Let $\mathscr{K}_k$, $\mathscr{H}_k$, H_k, B_k, A_k, $k = 0, 1$, and V and J be as defined above. Suppose that the wave operators $\Omega^{\pm}(V^{-1}B_1 V, B_0)$ exist (respectively, exist and are complete) on $\mathscr{K}_0$. Then the generalized wave operators $\Omega^{\pm}(A_1, A_0; J)$ exist (respectively, exist and are complete) and are partial isometries from $\mathscr{H}_0$ to $\mathscr{H}_1$ with initial space $P_{\text{ac}}(A_0)\mathscr{H}_0$.

Proof Since

$$\begin{aligned}\|J\langle u, v\rangle\|_{\mathscr{H}_1}^2 &= \|B_1(B_1^{-1}VB_0)u\|_{\mathscr{K}_1}^2 + \|Vv\|_{\mathscr{K}_1}^2\\ &= \|B_0 u\|_{\mathscr{K}_0}^2 + \|v\|_{\mathscr{K}_0}^2\\ &= \|\langle u, v\rangle\|_{\mathscr{H}_0}^2\end{aligned}$$

J is unitary and thus $\Omega^{\pm}(A_1, A_0; J)$ are partial isometries when they exist. The proof of the main statement of the theorem relies on the factorization

$$\frac{d^2}{dt^2} + B^2 = \left(\frac{d}{dt} - iB\right)\left(\frac{d}{dt} + iB\right)$$

so that if u obeys $u'' = -B^2 u$, then $f_{\pm} = u' \pm iBu$ obey $df_{\pm}/dt = \pm iBf_{\pm}$. To make the decomposition precise, we define

$$T_k = \frac{1}{\sqrt{2}}\begin{pmatrix} B_k & i \\ B_k & -i \end{pmatrix}$$

Then, by the parallelogram law, T_k is a unitary map of $\mathscr{H}_k$ onto $\mathscr{K}_k \oplus \mathscr{K}_k$ and

$$T_k A_k T_k^{-1} = \begin{pmatrix} B_k & 0 \\ 0 & -B_k \end{pmatrix}$$

Thus

$$T_k W_k(t) T_k^{-1} = \begin{pmatrix} e^{-iB_k t} & 0 \\ 0 & e^{iB_k t} \end{pmatrix} \equiv \tilde{W}_k(t)$$

Further, by multiplying out the matrices, one finds

$$T_1 J T_0^{-1} = \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} \equiv \tilde{V}$$

as a map from $\mathcal{K}_0 \oplus \mathcal{K}_0$ to $\mathcal{K}_1 \oplus \mathcal{K}_1$. Moreover, by Problem 112,

$$T_0 P_{\text{ac}}(A_0) = \begin{pmatrix} P_{\text{ac}}(B_0) & 0 \\ 0 & P_{\text{ac}}(B_0) \end{pmatrix} \equiv \tilde{P}_{\text{ac}}(B_0)$$

Now, for $\varphi \in \mathcal{H}_0$,

$$\begin{aligned} W_1(-t)JW_0(t)P_{\text{ac}}(A_0)\varphi &= T_1^{-1}\tilde{W}_1(-t)T_1 J T_0^{-1}\tilde{W}_0(t)T_0 P_{\text{ac}}(A_0)\varphi \\ &= T_1^{-1}\tilde{W}_1(-t)\tilde{V}\tilde{W}_0(t)\tilde{P}_{\text{ac}}(B_0)\varphi \\ &= (T_1^{-1}\tilde{V})(\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V})\tilde{W}_0(t)\tilde{P}_{\text{ac}}(B_0)\varphi \end{aligned}$$

Since

$$\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V} = \begin{pmatrix} e^{iV^{-1}B_1Vt} & 0 \\ 0 & e^{-iV^{-1}B_1Vt} \end{pmatrix}$$

we have

$$(\tilde{V}^{-1}\tilde{W}_1(-t)\tilde{V})\tilde{W}_0(t) = \begin{pmatrix} e^{iV^{-1}B_1Vt}e^{-iB_0t} & 0 \\ 0 & e^{-iV^{-1}B_1Vt}e^{iB_0t} \end{pmatrix}$$

Therefore $\lim_{t\to\pm\infty} W_1(-t)JW_0(t)P_{\text{ac}}(A_0)\varphi$ will exist for all $\varphi \in \mathcal{H}_0$ if and only if $\lim_{t\to\pm\infty} e^{iV^{-1}B_1Vt}e^{-iB_0t}P_{\text{ac}}(B_0)\psi$ exist for all $\psi \in \mathcal{K}_0$.

Since J is unitary, it is invertible. J^{-1} is automatically an A_0 left inverse of J and J is a A_1 left inverse of J^{-1}. Thus, according to Proposition 5c in Section 3, to show that $\Omega^{\pm}(A_1, A_0; J)$ are complete we need only show that $\Omega^{\pm}(A_0, A_1, J^{-1})$ exist. By a similar argument to the above, this is equivalent to the existence of the limits s-$\lim_{t\to\pm\infty} e^{iB_0t}e^{-iV^{-1}B_1Vt}P_{\text{ac}}(V^{-1}B_1V)$, which is equivalent to the completeness of $\Omega^{\pm}(V^{-1}B_1V, B_0)$ according to Proposition 3 of Section 3. ▌

It is clear from the above argument why J is such a convenient identification operator. However, from a physical point of view, J is artificial. For example, suppose that $\mathcal{K}_0$ and $\mathcal{K}_1$ are setwise equal with equivalent inner products, that the quadratic form domains of H_0 and H_1 are equal, and that

$$d_0(u, H_0u)_{\mathcal{K}_0} \le (u, H_1u)_{\mathcal{K}_1} \le d_1(u, H_0u)_{\mathcal{K}_0} \tag{193}$$

Equivalently,

$$d_0\|B_0u\|^2_{\mathcal{K}_0} \le \|B_1u\|^2_{\mathcal{K}_1} \le d_1\|B_0u\|^2_{\mathcal{K}_0}$$

so $\mathcal{H}_0$ and $\mathcal{H}_1$ are setwise equal with equivalent inner products. In this situation (which holds in the example of acoustic scattering), it is natural to use the identity $I_{01}\colon \mathscr{H}_0 \to \mathscr{H}_1$ as identification operator, and to ask about the existence and completeness of $\Omega^\pm(A_1, A_0, I_{01})$. We use the pedantic symbol I_{01} because we shall later consider I_{01}^* which is not equal to I_{10}. Suppose that a unitary $V\colon \mathscr{K}_0 \to \mathscr{K}_1$ is given and that we know from Theorem XI.75 that $\Omega^\pm(A_1, A_0; J)$ exist. If J and I_{01} are asymptotically A_0-equivalent, that is, if

$$\lim_{t\to\pm\infty} (J - I_{01})W_0(t)P_{\mathrm{ac}}^0(A_0)\varphi = 0 \tag{194}$$

for all $\varphi \in \mathscr{H}_0$, then according to Proposition 5a of Section 3, $\Omega^\pm(A_1, A_0; I_{01})$ exist and equal $\Omega^\pm(A_1, A_0, J)$. Since $J\langle u, v\rangle = \langle B_1^{-1}VB_0 u, Vv\rangle$, we expect (194) to hold only if V behaves B_0-asymptotically like the identity operator and B_0 and B_1 are asymptotically equal. Technically, we formulate the second condition by requiring that

$$\|(H_0 - V^{-1}H_1 V)e^{-iB_0t}w\|_{\mathscr{K}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty \tag{195}$$

for all w in a dense set $\mathscr{D} \subset D(H_0) \cap D(V^{-1}H_1 V) \cap P_{\mathrm{ac}}(H_0)$ that is invariant under e^{itB_0}, B_0, and B_0^{-1}. The first condition is met by requiring that

$$\|(I + V^{-1}H_1 V)(V^{-1} - I)e^{-iB_0t}w\|_{\mathscr{K}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty \tag{196}$$

for all $w \in \mathscr{D}$.

Theorem XI.76 Let $\mathscr{K}_k$, $\mathscr{H}_k$, H_k, B_k, A_k, $k = 0, 1$, V, J, and I_{01} be as defined above. Suppose that:

(i) $\mathscr{K}_0$ and $\mathscr{K}_1$ are setwise equal with equivalent inner products.
(ii) $Q(H_0) = Q(H_1)$ setwise and that (193) holds.
(iii) (195) and (196) hold.
(iv) The wave operators $\Omega^\pm(V^{-1}B_1 V, B_0)$ exist on $\mathscr{K}_0$.

Then (194) holds, so, in particular, $\Omega^\pm(A_1, A_0; I_{01})$ exist and equal $\Omega^\pm(A_1, A_0; J)$.

Proof Let w_0 and w_1 be in $\mathscr{D}$ and set $\varphi = \langle w_0, w_1\rangle$. Since $\mathscr{D}$ is dense in $P_{\mathrm{ac}}(H_0)$ and $(I_{01} - J)W_0(t)$ are uniformly bounded, it is sufficient to prove (194) for such φ. Let $u_0(t)$ and $v_0(t)$ be the components of $W_0(t)\varphi$. Then, since $\varphi \in P_{\mathrm{ac}}(A_0)$, we have

$$\begin{aligned}
&\|(J - I_{01})W_0(t)P_{\mathrm{ac}}(A_0)\varphi\|_{\mathscr{H}_1}^2 \\
&\quad = \|B_1(B_1^{-1}VB_0 - I)u_0(t)\|_{\mathscr{K}_1}^2 + \|(V - I)v_0(t)\|_{\mathscr{K}_1}^2 \\
&\quad = \|(B_0 - V^{-1}B_1)u_0(t)\|_{\mathscr{K}_0}^2 + \|(I - V^{-1})v_0(t)\|_{\mathscr{K}_0}^2
\end{aligned}$$

Since $v_0(t) = -B_0(\sin B_0 t)w_0 + (\cos B_0 t)w_1$ and $w_k \in \mathscr{D}$, (196) and the positivity of H_1 imply that the second term goes to zero as $t \to \pm\infty$. We estimate the first term by

$$\|(B_0 - V^{-1}B_1)u_0(t)\|_{\mathscr{H}_0}$$
$$\leq \|(B_0 - V^{-1}B_1 V)u_0(t)\|_{\mathscr{H}_0} + \|(V^{-1}B_1 V)(I - V^{-1})u_0(t)\|_{\mathscr{H}_0}$$

As above, the second term goes to zero by (196). For notational simplicity, set $B_1' = V^{-1}B_1 V$ and denote $\Omega^{\pm}(B_1', B_0)$ simply by $\Omega^{\pm}$. We must show that

$$\|(B_0 - B_1')e^{-itB_0}w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

or equivalently

$$\|e^{itB_1'}(B_0 - B_1')e^{-itB_0}w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

for w in $\mathscr{D}$. By (iv),

$$e^{iB_1't}B_0 e^{-iB_0t}w \to \Omega^+ B_0 w \qquad \text{as} \quad t \to -\infty$$

Thus, to conclude the result in the case $t \to -\infty$, it is sufficient to show that

$$e^{iB_1't}B_1' e^{-iB_0t}w = B_1' e^{iB_1't}e^{-iB_0t}w \to B_1'\Omega^+ w$$

since $B_1'\Omega_+ w = \Omega_+ B_0 w$. If we take $w \in \mathscr{D}$ and expand

$$\begin{aligned}\|B_1' e^{iB_1't}e^{-iB_0t}w - B_1'\Omega^+ w\|_{\mathscr{H}_0}^2 = {} & \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 + \|B_1'\Omega^+ w\|_{\mathscr{H}_0}^2 \\ & - (B_1' e^{iB_1't}e^{-iB_0t}w, B_1'\Omega^+ w)_{\mathscr{H}_0} \\ & - (B_1'\Omega^+ w, B_1' e^{iB_1't}e^{-iB_0t}w)_{\mathscr{H}_0}\end{aligned}$$

we see that, by taking B_1' to the other side, the last two terms converge to $-\|B_1'\Omega_+ w\|_{\mathscr{H}_0}^2$. Thus, to show that the whole expression goes to zero we need just prove that

$$\lim_{t \to -\infty} \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 \leq \|B_1'\Omega^+ w\|_{\mathscr{H}_0}^2$$

We compute,

$$\begin{aligned}\overline{\lim_{t \to -\infty}} \|B_1' e^{iB_1't}e^{-iB_0t}w\|_{\mathscr{H}_0}^2 &= \overline{\lim_{t \to -\infty}} (e^{-iB_0t}w, H_1' e^{-iB_0t}w)_{\mathscr{H}_0} \\ &= \overline{\lim_{t \to -\infty}} (e^{-iB_0t}w, H_0 e^{-iB_0t}w)_{\mathscr{H}_0} \\ &= \|B_0 w\|_{\mathscr{H}_0}^2 \\ &= \|\Omega_+ B_0 w\|_{\mathscr{H}_0}^2 \\ &= \|B_1'\Omega_+ w\|_{\mathscr{H}_0}^2 \end{aligned} \tag{197}$$

In the second step we used (195). This proves (194) in the case $t \to -\infty$. The other case is similar. ▮

Notice that all the hypotheses in Theorems XI.75 and XI.76 deal with H_0 and $H_1' = V^{-1}H_1V$ on $\mathcal{K}_0$. Thus the two Hilbert space scattering problem on $\mathscr{H}_0$ and $\mathscr{H}_1$ is reduced to studying the scattering theory for two self-adjoint operators on a single Hilbert space $\mathcal{K}_0$. In fact, if we changed our point of view slightly, we could reformulate Theorems XI.75 and XI.76 to avoid the two Hilbert space scattering theory entirely. For, if hypotheses (i) and (ii) of Theorem XI.76 hold, then $W_1(t)$ is a strongly continuous group of bounded operators on $\mathscr{H}_0$ (in general, not a unitary group). Hypotheses (iii) and (iv) give conditions on H_0 and $V^{-1}H_1V$ on $\mathcal{K}_0$ so that the "wave operators"

$$\underset{t \to \mp\infty}{\text{s-lim}}\ W_1(-t)W_0(t)P_{\text{ac}}(A_0)$$

exist on $\mathscr{H}_0$. And, according to Theorem XI.75, if $\Omega^{\pm}(V^{-1}H_1V, H_0)$ are complete, then these wave operators are complete as maps from $\mathscr{H}_0$ to $\mathscr{H}_0$.

Example 1, continued We can now apply these theorems to acoustic scattering. In addition to hypotheses (188) and (190) we assume that $c(x)$ and $\rho(x)$ are twice continuously differentiable with bounded derivatives. These smoothness assumptions can be avoided; see the discussion at the end of the section. We define $\mathcal{K}_0 = L^2(\mathbb{R}^3) = \mathcal{K}_1$ with inner products

$$(u, v)_{\mathcal{K}_0} = (c_0^2\rho_0)^{-1}(u, v)_{L^2(\mathbb{R}^3)}$$

$$(u, v)_{\mathcal{K}_1} = (u, (c(x)^2\rho(x))^{-1}v)_{L^2(\mathbb{R}^3)}$$

The operators H_k, B_k, and A_k are as described in Example 1. In particular, $D(B_0) = D(B_1)$ and (193) holds. Thus conditions (i) and (ii) of Theorem XI.76 hold, so the Hilbert spaces $\mathscr{H}_0$ and $\mathscr{H}_1$ constructed from $\mathcal{K}_0$ and $\mathcal{K}_1$ as above are setwise equal with equivalent inner products. We naturally choose V to be the unitary map $V\colon \mathcal{K}_0 \to \mathcal{K}_1$ given by

$$V\colon u(x) \mapsto [c(x)^2\rho(x)/c_0^2\rho_0]^{1/2}u(x)$$

so

$$V^{-1}H_1V = -[c(x)^2\rho(x)]^{1/2}(\nabla \cdot \rho(x)^{-1}\nabla)[c(x)^2\rho(x)]^{1/2}$$

To verify (195) and (196), we choose $\mathscr{D}$ to be the set of $f \in \mathscr{S}(\mathbb{R}^3)$ whose Fourier transforms have support away from the origin. Notice that $(H_0 - V^{-1}H_1V)e^{-iB_0t}w$ and $(I + V^{-1}H_1V)(V^{-1} - I)e^{-iB_0t}w$ can both be written as sums of terms of the form

$$f(x)e^{\pm iB_0t}P(D)w$$

where $P(D)$ is a constant coefficient partial differential operator and $f(x)$ is a product of terms of the form $\rho(x) - \rho_0$, $c(x) - c_0$, $\rho(x)$, ρ_0, $c(x)$, c_0, or their inverses or square roots, or their derivatives up to order two. Moreover, at least one factor of $\rho(x) - \rho_0$, $c(x) - c_0$, $D^\alpha \rho(x)$, or $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, occurs. For $w \in \mathscr{D}$, $e^{\pm iB_0 t} P(D) w$ is a regular wave packet for the free wave equation ($m = 0$) in three dimensions, so by Theorem XI.18,

$$\|e^{\pm iB_0 t} P(D) w\|_\infty \leq c/|t|$$

Thus, if we require that $\rho(x) - \rho_0$, $c(x) - c_0$, $D^\alpha \rho(x)$, $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, be in $L^2(\mathbb{R}^3)$, then

$$\|f(x) e^{\pm iB_0 t} P(D) w\|_{\mathscr{H}_0} \to 0 \qquad \text{as} \quad t \to \pm\infty$$

for each of the terms, so (195) and (196) hold. An alternative proof which avoids stationary phase ideas is as follows: Since $\hat{w}$ has compact support, $E_{[-M, M]}(-\Delta) w = w$ for some M. Thus if $\rho(x) - \rho_0$, etc. are in $L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$, then $f(x) E_{[-M, M]}(-\Delta)$ is Hilbert–Schmidt and thus compact. The convergence to zero then follows from Lemma 2 in Section 3.

It remains to investigate when $\Omega^\pm(V^{-1} B_1 V, B_0)$ exist and are complete. We first apply Theorem XI.10 (Birman's theorem) to $V^{-1} H_1 V$ and H_0. We already know that $D(B_1) = D(B_0)$, and, by the hypotheses on $\rho(x)$ and $c(x)$, $Q(H_0) = Q(V^{-1} H_0 V)$. Thus $D(V^{-1} B_1 V) = D(B_0)$, so $V^{-1} H_1 V$ and H_0 are mutually subordinate. Furthermore,

$$H_0 - V^{-1} H_1 V = (c(x)^2 - c_0^2)\, \Delta + h(x) \cdot \nabla + e(x)$$

where $h(x)$ and $e(x)$ are sums of functions of the form of $f(x)$ described above. Thus for each bounded interval I,

$$(H_0 - V^{-1} H_1 V) E_I(H_0)$$

is a sum of operators of the form

$$f(x) g(-i\nabla)$$

where g is the product of a polynomial and the characteristic function of a finite interval. According to Theorem XI.21, $f(x) g(-i\nabla)$ will be trace class if $f \in L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$. And, if $(H_0 - V^{-1} H_1 V) E_I(H_0)$ is trace class, then $E_I(V^{-1} H_1 V)(H_0 - V^{-1} H_1 V) E_I(H_0)$ is automatically trace class since $E_I(V^{-1} H_1 V)$ is bounded, so the conditions of Birman's theorem are fulfilled.

We have shown that if $c(x)^2 - c_0^2$, $\rho(x) - \rho_0$, $D^\alpha \rho(x)$, $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, are in $L^2_\delta(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$, then $\Omega^\pm(V^{-1} H_1 V, H_0)$ exist and are complete. Since $\sqrt{x}$ is an admissible function, the invariance principle (Theorem XI.11) implies that $\Omega^\pm(V^{-1} B_1 V, B_0)$ exist and are complete. Thus, applying Theorems XI.75 and XI.76 we have:

Theorem XI.77 Suppose that $c(x)$ and $\rho(x)$ are twice continuously differentiable functions with bounded derivatives satisfying (188) and (190). Suppose that $c(x)^2 - c_0^2$, $\rho(x) - \rho_0$, $D^\alpha \rho(x)$, $D^\alpha c(x)$, $0 \neq |\alpha| \leq 2$, are all in $L_\delta^2(\mathbb{R}^3)$ for some $\delta > \frac{3}{2}$. Then, the wave operators $\Omega^\pm(A_1, A_0; I_{01})$ associated with the systems (186), (187) exist and are complete.

We have proven completeness in the sense of generalized wave operators. It can be proven that $\mathscr{H}_{\text{ac}}(A_1) = \mathscr{H}_1$, so *every* solution of (187) is asymptotic to a free solution. We have essentially proven that A_1 has no singular continuous spectrum in the appendix to Section 6. We shall prove that A_1 has no eigenvalues in Section XIII.13.

The decay conditions on $c(x)^2 - c_0^2$, $\rho(x) - \rho_0$, $D^\alpha \rho(x)$, $D^\alpha c(x)$ are not very stringent in that they will hold in any reasonable physical situation. On the other hand, the smoothness hypotheses restrict the applicability of the theorem greatly since in many inhomogeneous media problems there is a sudden change in $\rho(x)$ or $c(x)$ as one passes from one medium to the next. Fortunately, the smoothness hypotheses can be removed.

Example 1, revisited Existence and completeness of the wave operators for acoustical scattering in an inhomogeneous medium can also be proven by applying the Birman–Belopol'skii theorem (Theorem XI.13) directly. We take $\mathscr{K}_k$, $\mathscr{H}_k$, A_k, H_k, and B_k to be as above and choose I_{01} as the identification operator from $\mathscr{H}_0$ to $\mathscr{H}_1$. We must verify that hypotheses (a)–(d) of Theorem XI.13 hold. (a) is obvious. Since $D(A_k) = D(B_k^2) \oplus D(B_k)$ and we already know that $D(B_0) = D(B_1)$, we need only prove that $D(H_0) = D(H_1)$ to conclude that (d_1) holds. And, since V takes $D(H_0)$ into itself, we need only prove that $V^{-1} H_1 V$ and H_0 have the same domain on $\mathscr{K}_0$. The proof, which uses the symmetric form of the Kato–Rellich theorem (see Problem 66), is left to the reader.

To prove condition (b), we want to show that $(A_1 - A_0)E_I(A_0)$ is trace class as an operator from $\mathscr{H}_0$ to $\mathscr{H}_1$. Since the identity is bounded from $\mathscr{H}_0$ to $\mathscr{H}_1$, it is sufficient to show that $(A_1 - A_0)E_I(A_0)$ is trace class as an operator on $\mathscr{H}_0$. Set $C = B_0^2 - B_1^2$ and let T_0 be the unitary map $T_0 \colon \mathscr{H}_0 \to \mathscr{K}_0 \oplus \mathscr{K}_0$ introduced in the proof of Theorem XI.75. Then

$$T_0(A_1 - A_0)E_I(A_0)T_0^{-1} = \frac{1}{2}\begin{pmatrix} -CB_0^{-1} & -CB_0^{-1} \\ CB_0^{-1} & CB_0^{-1} \end{pmatrix}\begin{pmatrix} E_I(B_0) & 0 \\ 0 & E_I(B_0) \end{pmatrix}$$

on $\mathscr{K}_0 \oplus \mathscr{K}_0 = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. Since ∇B_0^{-1} is a bounded operator commuting with $E_I(B_0)$, the same proof as in Example 1 (continued) shows that $\pm CB_0^{-1}E_I(B_0)$ is trace class on $L^2(\mathbb{R}^3)$ if the conditions on $c(x)$ and $\rho(x)$

expressed in Theorem XI.77 hold. Therefore (b) holds under these conditions.

Finally, we must check (c). An easy calculation shows that $I_{01}^*: \mathscr{H}_1 \to \mathscr{H}_0$ is given by

$$I_{01}^*\langle u, v\rangle = \langle -(c_0^2\rho_0)B_0^{-2}\nabla \cdot \rho(x)^{-1}\nabla u, (c_0^2\rho_0/c(x)^2\rho(x))v\rangle$$

Thus, we may write

$$(I_{01}^* I_{01} - I_{00})\langle u, v\rangle = \langle Q_1 u, Q_2 v\rangle$$

where

$$Q_1 = -(c_0^2\rho_0)B_0^{-2}\nabla \cdot (1/\rho(x))\nabla - I$$

$$Q_2 = (c_0^2\rho_0/c(x)^2\rho(x)) - I$$

Using the diagonalizing transformation T_0 as above, we find that

$$T_0(I_{01}^* I_{01} - I_{00})E_I(A_0)T_0^{-1}$$
$$= \frac{1}{2}\begin{pmatrix} B_0 Q_1 B_0^{-1} + Q_2 & B_0 Q_1 B_0^{-1} - Q_2 \\ B_0 Q_1 B_0^{-1} - Q_2 & B_0 Q_1 B_0^{-1} + Q_2 \end{pmatrix}\begin{pmatrix} E_I(B_0) & 0 \\ 0 & E_I(B_0) \end{pmatrix}$$

Thus, we are reduced to showing that $B_0 Q_1 B_0^{-1}E_I(B_0)$ and $Q_2 E_I(B_0)$ are compact as operators on $L^2(\mathbb{R}^3)$. For the second operator, this follows immediately if $c(x)$ and $\rho(x)$ obey the conditions of Theorem XI.77. For the first operator, notice that

$$B_0 Q_1 B_0^{-1}E_I(B_0) = -(c_0^2\rho_0)(B_0^{-1}\nabla) \cdot \left(\frac{1}{\rho(x)} - \frac{1}{\rho_0}\right)(\nabla B_0^{-1})E_I(B_0)$$

Since $B_0^{-1}\nabla$ is bounded and $(\rho(x)^{-1} - \rho_0^{-1})(\nabla B_0^{-1})E_I(B_0)$ is trace class by Theorem XI.21, $B_0 Q_1 B_0^{-1}E_I(B_0)$ is trace class and therefore compact. We conclude that $(I_{01}^* I_{01} - I_{00})E_I(A_0)$ is compact if $\rho(x)$ satisfies the conditions of Theorem XI.77.

We have verified conditions (a)–(d_1) of the Birman–Belopol'skii theorem, so the wave operators $\Omega^\pm(A_1, A_0; I)$ exist and are complete. Notice that using the Birman–Belopol'skii theorem does not avoid completely the reduction to a single Hilbert space since we must make the reduction to verify the hypotheses. The reason that we have avoided explicit proof of (195) and (196) is that we have used a compactness argument, as we could have in the verification of (195) and (196).

Example 2 (optical scattering) The scattering of electromagnetic waves in an inhomogeneous medium is governed by Maxwell's equations:

$$\begin{aligned} \nabla \times E &= -\mu(x) \frac{\partial H}{\partial t} & \nabla \times H &= \varepsilon(x) \frac{\partial E}{\partial t} \\ \nabla \cdot (\varepsilon(x)E) &= 0 & \nabla \cdot (\mu(x)H) &= 0 \end{aligned} \tag{198}$$

E and H are functions from $\mathbb{R}^3$ to $\mathbb{R}^3$ representing the electric and magnetic fields. $\varepsilon(x)$ and $\mu(x)$ are three-by-three matrix-valued functions on $\mathbb{R}^3$ representing the dielectric and magnetic susceptibilities. We assume that $\varepsilon(x)$ and $\mu(x)$ are C^2 with bounded derivatives; and since we want the energy

$$(E, H) = \int_{\mathbb{R}^3} [\overline{E(x)} \cdot \varepsilon(x)E(x) + \overline{H(x)} \cdot \mu(x)H(x)]\, dx$$

to be positive, we require that

$$c_1 I \le \varepsilon(x) \le c_2 I, \qquad c_3 I \le \mu(x) \le c_4 I \tag{199}$$

for all x for some positive constants c_i. Suppose that there are constant positive definite matrices ε_0 and μ_0 so that

$$\varepsilon(x) \to \varepsilon_0, \qquad \mu(x) \to \mu_0$$

as $|x| \to \infty$. Then we should be able to develop a scattering theory for (198) in terms of the free equations

$$\begin{aligned} \nabla \times E &= -\mu_0 \frac{\partial H}{\partial t} & \nabla \times H &= \varepsilon_0 \frac{\partial E}{\partial t} \\ \nabla \cdot (\varepsilon_0 E) &= 0 & \nabla \cdot (\mu_0 H) &= 0 \end{aligned} \tag{200}$$

In order to do this we rewrite (198) as a second-order equation for E:

$$\ddot{E} = -\varepsilon^{-1} \nabla \times (\mu^{-1}(\nabla \times E)) \tag{201}$$

and similarly for (200). Now, define $\mathscr{H}_0$ and $\mathscr{H}_1$ to be $L^2(\mathbb{R}^3)^3$ with inner products

$$(E, F)_{\mathscr{H}_0} \equiv \int_{\mathbb{R}^3} \overline{E(x)} \cdot \varepsilon_0 F(x)\, dx$$

$$(E, F)_{\mathscr{H}_1} \equiv \int_{\mathbb{R}^3} \overline{E(x)} \cdot \varepsilon(x) F(x)\, dx$$

Let $\mathscr{Q} = \{E \in L^2(\mathbb{R}^3)^3 \mid \nabla \times E \in (L^2)^3\}$ and define quadratic forms q_0 and q_1 on $\mathscr{Q}$ by

$$q_0(E, F) = \int_{\mathbb{R}^3} (\nabla \times E) \cdot \mu_0^{-1}(\nabla \times F)\, dx$$

$$q_1(E, F) = \int_{\mathbb{R}^3} (\nabla \times E) \cdot \mu(x)^{-1}(\nabla \times F)\, dx$$

q_0 and q_1 are the quadratic forms of positive self-adjoint operators on $\mathscr{H}_0$ and $\mathscr{H}_1$, respectively,

$$H_0 E = -\varepsilon_0^{-1}\nabla \times \mu_0^{-1}(\nabla \times E)$$
$$H_1 E = -\varepsilon(x)^{-1}\nabla \times \mu(x)^{-1}(\nabla \times E)$$

and the square roots of these operators satisfy (193) because of (199). Finally, we define $V\colon \mathscr{H}_0 \to \mathscr{H}_1$ by

$$(VE)(x) = \varepsilon(x)^{-1/2}\varepsilon_0^{1/2}E(x)$$

We are thus in the situation covered by Theorems XI.75 and XI.76 except that H_0 and H_1 have point spectrum at zero. This does not cause any difficulty in these theorems for they can easily be extended to handle this case; see the reference in the Notes. Thus, as in Example 1, the scattering problem can be reduced to studying H_0 and $V^{-1}H_1 V$ on $\mathscr{H}_0$. (195) and (196) follow as in Example 1 since $P_{\mathrm{ac}}(H_0)$ projects out the zero modes and each component of $e^{\pm iB_0 t}P_{\mathrm{ac}}(B_0)w$ obeys a free wave equation and thus satisfies

$$\|e^{\pm iB_0 t}P_{\mathrm{ac}}(B_0)w\|_\infty < c/t$$

Using this estimate, stationary phase, and Cook's method, one can easily show that the wave operators $\Omega^\pm(V^{-1}H_1 V, H_0)$ exist. Thus one obtains the existence of $\Omega^\pm(A_1, A_0; I_{01})$ analogously to Example 1.

The zero modes do cause a new difficulty in the proof of completeness, however, since one can no longer expect

$$(V^{-1}H_1 V - H_0)E_I(H_0)$$

to be trace class when the interval I contains zero. One possible way out would be to try to prove the existence of the limits

$$e^{iH_0 t}e^{-iV^{-1}H_1 V t}P_{\mathrm{ac}}(V^{-1}H_1 V)w$$

directly by using Cook's method. But this is very difficult since

$$e^{-iV^{-1}H_1 V t}P_{\mathrm{ac}}(V^{-1}H_1 V)w$$

will satisfy a wave equation with nonconstant coefficients and thus one cannot use the Fourier transform to prove estimates. Instead, one gets around the difficulty as follows. Define operators $\tilde{H}_k$ on $\mathscr{H}_k$ by the quadratic forms

$$\tilde{q}_k(E, F) = q_k(E, F) + \int (\nabla \cdot \gamma_k E) \cdot (\nabla \cdot \gamma_k F)\, dx$$

where $\gamma_0 = \varepsilon_0$ and $\gamma_1 = \varepsilon(x)$. One can prove that

$$(V^{-1}\tilde{H}_1 V + 1)^{-2} - (\tilde{H}_0 + 1)^{-2}$$

is trace class, essentially because the addition of the extra term has removed the zero modes and made $V^{-1}\tilde{H}_1 V$ and $\tilde{H}_0$ strictly elliptic. The existence and completeness of $\Omega^{\pm}(V^{-1}\tilde{H}_1 V, \tilde{H}_0)$ then follows from Corollary 2 of Theorem XI.11. Finally, one shows by an elementary argument that the existence of $\Omega^{\pm}(\tilde{H}_0, V^{-1}\tilde{H}_1 V)$ implies the existence of $\Omega^{\pm}(H_0, V^{-1}H_1 V)$. The reason is that the dynamical modes and the zero modes are completely decoupled in Maxwell's equations, so giving a spurious dynamics to the zero modes does not affect the dynamical modes. For details, see the reference in the Notes.

Example 3 (scattering of acoustical waves from obstacles) Let $\mathcal{O}$ be a closed bounded set in $\mathbb{R}^3$ whose boundary Γ has measure zero and whose complement is connected. Then the acoustic wave equation in the exterior of the obstacle $\mathcal{O}$ is

$$\begin{aligned} u_{tt} - \Delta u &= 0, && x \in \mathbb{R}^3\backslash\mathcal{O} \\ \frac{\partial u}{\partial \hat{n}} &= 0, && x \in \Gamma \\ u(x, 0) &= f(x), && x \in \mathbb{R}^3\backslash\mathcal{O} \\ u_t(x, 0) &= g(x), && x \in \mathbb{R}^3\backslash\mathcal{O} \end{aligned} \tag{202}$$

where u is the difference between the pressure at x at time t and the equilibrium pressure. The Neumann boundary conditions can be understood as follows: A pressure gradient causes a proportional fluid flow. Thus the condition $\nabla u \cdot \hat{n} = 0$ on Γ just says that there is no flow across Γ. Given an initial disturbance $\langle f(x), g(x)\rangle$ exterior to the obstacle, the solution of (202) will depend on the geometry of the obstacle; but for large positive and negative times, the waves should propagate away from the obstacle to infinity. As more and more of the energy goes away from the obstacle, the solution of (202) should look more and more like a solution of $u_{tt} - \Delta u = 0$

on all of $\mathbb{R}^3$. Thus, we expect to be able to construct a scattering theory for (202) in terms of the solutions of the free wave equation.

We can choose the same Hilbert space for H_0 and H_1 by the simple expedient of allowing the interior of the obstacle to have acoustic disturbances. Since the interior and the exterior are decoupled, this does not affect the scattering theory. Let H_0 denote $-\Delta$ on $L^2(\mathbb{R}^3)$ and let H_1 be the Neumann Laplacian H_{N} on $L^2(\mathbb{R}^3)$ with boundary Γ as defined in Section XIII.15. Thus in this case, we have $\mathcal{K}_0 = L^2(\mathbb{R}^3) = \mathcal{K}_1$ and because of the boundary conditions, $Q(H_{\mathrm{N}}) \supset Q(H_0)$. Further, for $w \in Q(H_0)$, we have

$$\|B_0 w\|_2^2 = \|B_{\mathrm{N}} w\|_2^2 \tag{203}$$

The only difficulty applying the abstract theory developed in Theorem XI.75 is that if Γ separates $\mathbb{R}^3$ into more than one connected component, then B_1 will have zero as an eigenvalue: $H_{\mathrm{N}}\varphi = 0$ and $\varphi \in L^2(\mathbb{R}^3)$ if φ is constant on one of the bounded connected components. Physically, these eigenfunctions are irrelevant to the problem since they are *interior* to the obstacle. Mathematically, one can overcome this difficulty by extending Theorem XI.75 so that it allows point spectrum at zero (see the reference in the Notes) or by the following simple expedient: We redefine H_{N} on each such internal constant eigenfunction φ so that $H_{\mathrm{N}}\varphi = \varphi$. Assuming that there are only finitely many connected internal components, this redefinition does not affect any of the trace class conditions mentioned below or proven in the appendix. Having redefined H_{N} in this way we can apply the theory developed in this section. In particular, by Theorem XI.75, $\Omega^{\pm}(A_{\mathrm{N}}, A_0; J)$ exist and are complete from $\mathcal{H}_0$ to $\mathcal{H}_1$ if $\Omega^{\pm}(H_{\mathrm{N}}, H_0)$ exist and are complete on $\mathcal{K}_0 = L^2(\mathbb{R}^3)$. Here $J\colon \langle u, v\rangle \mapsto \langle B_{\mathrm{N}}^{-1}B_0 u, v\rangle$. In the appendix we show how to prove that $(H_{\mathrm{N}}+1)^{-2} - (H_0+1)^{-2}$ is trace class and thus, by Corollary 3 of Theorem XI.11, $\Omega^{\pm}(H_{\mathrm{N}}, H_0)$ exist and are complete.

It is no longer true that $\mathcal{H}_0 = \mathcal{H}_1$ since (193) does not hold in this case. However, since $Q(H_0) \subset Q(H_{\mathrm{N}})$ and (203) holds, $\mathcal{H}_0$ can be naturally imbedded as a subspace of $\mathcal{H}_1$. Therefore, it is natural to choose this embedding as the identification operator. Notice that (193) is not used anywhere in the proof of Theorem XI.76 although it is needed to have $\mathcal{H}_0 = \mathcal{H}_1$. Since $V = I$, condition (196) holds automatically; and because of (203), condition (195) is not necessary. For the proof of Theorem XI.76 goes through as before except that the crucial equality (197) holds because of (203) without appealing to (193) and (195). Thus $\Omega^{\pm}(A_{\mathrm{N}}, A_0; I)$ exist and are complete.

The case of scattering from an obstacle with Dirichlet boundary conditions is less interesting physically; but because the corresponding local compactness result is simpler (see the appendix), it is a good test case for various approaches to scattering theory. Let $H_1 = H_D$, the Dirichlet Laplacian with boundary Γ as defined in Section XIII.15. Then $Q(H_D) \subset Q(H_0)$ and

$$\|B_0 w\|_2^2 = \|B_D w\|_2^2 \tag{204}$$

for $w \in Q(H_D)$. Thus we have a similar setup to the one above except that $Q(H_D) \subset Q(H_0)$, whereas in the Neumann case $Q(H_N) \supset Q(H_0)$. Therefore we deal with the adjoints of the usual wave operators. Theorem XI.75 shows that $\Omega^\pm(A_0, A_D, J')$ exist and are complete as maps from $\mathscr{H}_1$ to $\mathscr{H}_0$ if $\Omega^\pm(H_0, H_D)$ exist and are complete on $\mathscr{K}_1 = L^2(\mathbb{R}^3)$. Here $J'\colon \langle u, v\rangle \mapsto \langle B_0^{-1} B_D u, v\rangle$. In the appendix we show that $(H_0 + 1)^{-2} - (H_D + 1)^{-2}$ is trace class so, as above, the existence and completeness of $\Omega^\pm(H_0, H_D)$ follow from Corollary 3 of Theorem XI.11. By the same idea described above, the conclusions of Theorem XI.76 follow automatically from (204), so J' may be replaced by the embedding I_{10} taking $\mathscr{H}_1$ into $\mathscr{H}_0$. That is, $\Omega^\pm(A_0, A_D; I_{10})$ exist and are complete. Since I_{10} is an isometry, I_{10}^* is an A_D-left inverse for I_{10}. Thus, by Proposition 5c of Section 3, $\Omega^\pm(A_D, A_0; I_{10}^*)$ exist and are complete.

We have proven:

Theorem XI.78 Let $\mathcal{O}$ be a closed bounded set in $\mathbb{R}^3$ with boundary Γ.

(a) If Γ has measure zero, if $\mathbb{R}^3 \backslash \Gamma$ has finitely many connected components, and if Γ obeys the regularity condition of Theorem XI.81, then the wave operators for the equation (202) with Neumann boundary conditions exist and are complete.

(b) If Γ has measure zero, then the wave operators for (202) with Dirichlet boundary conditions exist and are complete.

In Examples 1 and 2 we assumed that the coefficients describing the inhomogeneity were C^2 functions of the space variables. This is a very restrictive condition since some of the most interesting physical problems involve sharp changes in wave velocities or densities when passing from one medium to another. Fortunately, one can handle the nonsmooth case without great difficulty. Notice that in Example 1 we did not use any smoothness of $\rho(x)$ in defining H_1 on $\mathscr{K}_1$ and, of course, no smoothness is used in the abstract theorems. The only place that we used smoothness was in verifying that $(V^{-1}H_1 V - H_0)E_I(H_0)$ is trace class on $L^2(\mathbb{R}^3)$; we needed to express $V^{-1}H_1 V - H_0$ as a sum of terms of the form $f(x)P(D)$, so we could apply Theorem XI.21. P. Deift has shown how to use the commutation formula

$$\frac{\lambda}{BA + \lambda} + B\frac{1}{AB + \lambda}A = 1 \tag{205}$$

to avoid this difficulty. If A and B are bounded operators on a Hilbert space $\mathscr{H}$, then $\sigma(AB)\backslash\{0\} = \sigma(BA)\backslash\{0\}$ and for $-\lambda \notin \sigma(AB) \cup \{0\}$, (205) holds. The reader is asked to provide a proof in Problem 115. More generally, if A is a closed operator and $B = A^*$, then (205) holds for $-\lambda \in \mathbb{C}\backslash[0, \infty)$. To see how to use (205), consider the one-dimensional case where the notation is the simplest. Then $H_1' = V^{-1}H_1V = -aDb^2Da$ and $H_0 = D^2$ where $D = i\,d/dx$ and a and b are functions of x satisfying

$$0 < a_0 \le a(x) \le a_1, \qquad 0 \le b_0 \le b(x) \le b_1$$

and we assume that $a(x) \to 1$, $b(x) \to 1$ sufficiently fast as $|x| \to \infty$. As in Example 1, we define H_1' as follows: Let Db^2D be the self-adjoint operator on $L^2(\mathbb{R})$ corresponding to the closure of the symmetric quadratic form $q(\varphi, \varphi) = (D\varphi, b^2D\varphi)_{L^2}$ on $C_0^\infty(\mathbb{R}) \times C_0^\infty(\mathbb{R})$. Since multiplication by a has a bounded inverse, $H_1' = aDb^2Da$ is a well-defined self-adjoint operator. We want to prove that

$$\frac{1}{aDb^2Da + 1} - \frac{1}{D^2 + 1}$$

is trace class. Using the formula

$$\frac{1}{aDb^2Da + 1} = a^{-1}\left(\frac{1}{Db^2D + a^{-2}}\right)a^{-1}$$

and the properties of a, this problem is easily reduced to proving that

$$\frac{1}{Db^2D + 1} - \frac{1}{D^2 + 1}$$

is trace class. Let A be the operator bD. Then since we defined Db^2D by using quadratic forms, $Db^2D = (bD)^*(bD)$ (see Section X.3) where bD denotes the operator closure of $bD \restriction C_0^\infty(\mathbb{R})$. Setting $B = (bD)^*$ and applying the commutation formula, we have

$$\begin{aligned}\frac{1}{(bD)^*(bD) + 1} &= 1 - (bD)^*\left(\frac{1}{(bD)(bD)^* + 1}\right)(bD)\\ &= 1 - D^*\left(\frac{1}{D^*D + b^{-2}}\right)D\end{aligned}$$

and hence

$$\frac{1}{Db^2D + 1} - \frac{1}{D^2 + 1} = D^*\left(\frac{1}{D^*D + 1} - \frac{1}{D^*D + b^{-2}}\right)D$$

Thus, one is reduced to studying

$$\frac{1}{D^*D+1}-\frac{1}{D^*D+1+(b^{-2}-1)}$$

which can be handled by the usual methods for dealing with perturbations of $-d^2/dx^2$ by a potential. Essentially, the commutation formula allows us to unwrap Db^2D and get the b's on the outside.

The ideas in the three-dimensional case (discussed in the reference in the Notes) are the same with two exceptions. $D = i\nabla$ so bD is an operator from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)^3$ and $(bD)^*$ is an operator from $L^2(\mathbb{R}^3)^3$ to $L^2(\mathbb{R}^3)$. Thus one extends the commutation formula to the case where A is a closed operator from one Hilbert space to another and $B = A^*$. Also it is necessary to deal with the squares of the resolvents.

If the discontinuities of a and b lie in a compact set, one can also study the problem by using the twisting trick of the appendix to Section XI.11.

Appendix to XI.10: Trace class properties of Green's functions

Let Γ be a closed bounded subset of measure zero in $\mathbb{R}^n$. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$ and let $H_{\Gamma;\mathrm{D}}$ and $H_{\Gamma;\mathrm{N}}$ be $-\Delta$ on $L^2(\mathbb{R}^n)$ with Dirichlet and Neumann boundary conditions on Γ as defined in Section XIII.15. Set $R_0 = (H_0+1)^{-1}$, $R_{\Gamma;\mathrm{D}} = (H_{\Gamma;\mathrm{D}}+1)^{-1}$, $R_{\Gamma;\mathrm{N}} = (H_{\Gamma;\mathrm{N}}+1)^{-1}$. In this appendix we shall prove that $R_0^2 - R_{\Gamma;\mathrm{D}}^2$ and $R_0^2 - R_{\Gamma;\mathrm{N}}^2$ are trace class under suitable hypotheses on Γ when $n = 3$. Similar methods work for $n \neq 3$ if R^2 is replaced by R^m where $m > \frac{1}{2}n$ (Problem 116). Applications of these methods to the scattering of acoustical waves from obstacles appear in Example 3 of this section.

The basic results are:

Theorem XI.79 Let Γ be an arbitrary closed bounded subset of measure zero in $\mathbb{R}^3$. Then $R_0^2 - R_{\Gamma;\mathrm{D}}^2$ is trace class.

Theorem XI.80 Let Γ be a closed bounded subset of measure zero in $\mathbb{R}^3$. Let B be an open ball containing Γ and let $\tilde{H}_{\partial B\cup\Gamma;\mathrm{N}}$ be $-\Delta$ on $L^2(B)$ with Neumann boundary conditions on $\Gamma \cup \partial B$. Set

$$\tilde{R}_{\partial B\cup\Gamma;\mathrm{N}} = (H_{\partial B\cup\Gamma;\mathrm{N}}+1)^{-1}$$

and suppose that $\tilde{R}_{\partial B\cup\Gamma;\mathrm{N}}^2$ is trace class. Then $R_0^2 - R_{\Gamma;\mathrm{N}}^2$ is trace class.

Notice that $R_0^2 - R_{\Gamma;\mathrm{D}}^2 \in \mathscr{I}_1$ for any Γ, but we need restrictions on Γ in the Neumann case. The following example shows that these restrictions are necessary:

Example Let Λ be the union of an infinite number of disjoint balls of smaller and smaller radii all within the unit ball and let $\Gamma = \partial\Lambda$. Then $H_{\Gamma;\mathrm{N}}$ has zero as an eigenvalue of infinite multiplicity and the corresponding eigenfunctions have support in the ball. If χ is multiplication by the characteristic function of the ball, then $\chi R_{\Gamma;\mathrm{N}}^m$ is not compact for any m. On the other hand χR_0^m is compact for any $m \geq 2$ by Theorem XI.21, so $R_0^m - R_{\Gamma;\mathrm{N}}^m$ is not compact for any m.

Of course, Theorem XI.80 is not very useful unless there are conditions that guarantee that $\tilde{R}_{\partial B \cup \Gamma;\mathrm{N}}^2$ is trace class. In fact, there are very general sufficient conditions:

Definition A **truncated cone at** $x \in \mathbb{R}^n$ is a set of the form

$$\{y \mid 0 < |y - x| < \varepsilon, (y - x) \cdot n > (1 - \delta)|y - x|\}$$

for some $\varepsilon, \delta > 0$ and some unit vector n. An open set $\Lambda \subset \mathbb{R}^n$ with bounded boundary is said to have the **restricted cone property** if and only if there is a finite open cover $U_1, \ldots, U_k$ of $\partial\Lambda$ and truncated cones $C_1, \ldots, C_k$ at 0 so that $C_i + x \subset \Lambda$ if $x \in U_i \cap \Lambda$.

It is not hard to see that polyhedra and sets with smooth boundary have the restricted cone property.

Theorem XI.81 Let Γ be a closed bounded set of measure zero in $\mathbb{R}^3$. Write $\mathbb{R}\backslash\Gamma = \Lambda_1 \cup \Lambda_2$ where Λ_1 is the unbounded component and Λ_2 the union of the bounded components. Suppose that Λ_1 and Λ_2 have the restricted cone property. Then for any open ball containing Γ, $\tilde{R}_{\partial B \cup \Gamma;\mathrm{N}}^2$ is trace class.

In this appendix we prove Theorems XI.79 and 80 and sketch a proof of Theorem XI.81 in the special case where Γ is the union of the boundaries of a finite number of starlike regions with smooth boundary. The general case of Theorem XI.81, which is proven by very different methods, can be found in the reference in the Notes.

In the proofs of Theorems XI.79 and 80, we need various properties of R_0, $R_{\Gamma;\mathrm{D}}$, $R_{\Gamma;\mathrm{N}}$ established in Chapter XIII or by the methods of that chapter. We summarize the results that we need:

Lemma 1 Let Γ be fixed and B be a fixed ball containing Γ. Then:

(a) As operator inequalities on $L^2(\mathbb{R}^3)$,

$$R_{\Gamma;\mathrm{D}} \le R_0 \le R_{\Gamma;\mathrm{N}} \le R_{\partial B \cup \Gamma;\mathrm{N}}$$

(b) Under the direct sum decomposition $L^2(\mathbb{R}^3) = L^2(B) \oplus L^2(\mathbb{R}^3 \backslash B)$, $R_{\partial B \cup \Gamma;\mathrm{N}} = \tilde{R}_{\partial B \cup \Gamma;\mathrm{N}} \oplus R'$ for suitable R'.

(c) R_0, $R_{\Gamma;\mathrm{D}}$, and $R_{\Gamma;\mathrm{N}}$ are contractions from $L^\infty(\mathbb{R}^3)$ to itself.

Proof (a) In a suitable sense of $\le$ for unbounded operators, $H_{\Gamma \cup \partial B;\mathrm{N}} \le H_{\Gamma;\mathrm{N}} \le H_0 \le H_{\Gamma;\mathrm{D}}$ (see Proposition 4 of Section XIII.15) from which (a) follows by general principles (Problem 117).

(b) This is just Proposition 3 of Section XIII.15.

(c) By the second Beurling–Deny criterion (Theorem XIII.51), $e^{-tH_{\Gamma;\mathrm{D}}}$ is a contraction on L^∞ (see Example 3, revisited, in Appendix 1 to Section XIII.12) and thus since

$$R_{\Gamma;\mathrm{D}} = \int_0^\infty e^{-t} e^{-tH_{\Gamma;\mathrm{D}}}\, dt$$

so is $R_{\Gamma;\mathrm{D}}$. A similar proof works for R_0 and $R_{\Gamma;\mathrm{N}}$. ∎

Lemma 2 If $(1 + x^2)(R_0 - R_{\Gamma;\mathrm{D}})(1 + x^2)$ is Hilbert–Schmidt, then $R_0^2 - R_{\Gamma;\mathrm{D}}^2$ is trace class. Similarly, if $(1 + x^2)(R_0 - R_{\Gamma;\mathrm{N}})(1 + x^2)$ is Hilbert–Schmidt, then $R_0^2 - R_{\Gamma;\mathrm{N}}^2$ is trace class.

Proof Write

$$R_0^2 - R_{\Gamma;\mathrm{D}}^2 = R_0(R_0 - R_{\Gamma;\mathrm{D}}) + (R_0 - R_{\Gamma;\mathrm{D}})R_0 - (R_0 - R_{\Gamma;\mathrm{D}})^2$$

By Theorem XI.21 or by explicit calculation from the integral kernel $4\pi|x - y|^{-1}e^{-|x-y|}$ of R_0, $R_0(1 + x^2)^{-1}$ is Hilbert–Schmidt. Thus, to prove that $R_0^2 - R_{\Gamma;\mathrm{D}}^2$ is trace class, it suffices that $(1 + x^2)\,(R_0 - R_{\Gamma;\mathrm{D}})$ and $(R_0 - R_{\Gamma;\mathrm{D}})$ be Hilbert–Schmidt and this follows from the hypotheses. The Neumann case is similar. ∎

Lemma 3 Let $K \ge 0$ and let C and D be bounded operators with $C + D = I$. Then K is Hilbert–Schmidt if and only if C^*KC and D^*KD are Hilbert–Schmidt. In particular, if χ is the characteristic function of a bounded set Ω and both

$$\chi(R_0 - R_{\Gamma;\mathrm{D}})\chi \qquad \text{and} \qquad (1 + x^2)(1 - \chi)(R_0 - R_{\Gamma;\mathrm{D}})(1 - \chi)(1 + x^2)$$

respectively,

$$\chi(R_{\Gamma;\mathrm{N}} - R_0)\chi \qquad \text{and} \qquad (1 + x^2)(1 - \chi)(R_{\Gamma;\mathrm{N}} - R_0)(1 - \chi)(1 + x^2)$$

are Hilbert–Schmidt, then $R_0^2 - R_{\Gamma;\mathrm{D}}^2$ [respectively, $(R_0^2 - R_{\Gamma;\mathrm{N}}^2)$] is trace class.

Proof For K to be in $\mathscr{I}_2$, it is necessary and sufficient that $K^{1/2}$ be in $\mathscr{I}_4$. But this happens if and only if both $K^{1/2}C$ and $K^{1/2}D$ are in $\mathscr{I}_4$. This proves the first part of the lemma.

The last part of the lemma follows from the first part, Lemma 2 and Lemma 1a, which implies that $R_{\Gamma;\mathrm{N}} - R_0$ and $R_0 - R_{\Gamma;\mathrm{D}}$ are nonnegative operators. ▮

$R_{\Gamma;\mathrm{D}}$ defines a bilinear form on $\mathscr{S} \times \mathscr{S}$ by $\langle \varphi, \psi \rangle \mapsto (\bar{\varphi}, R_{\Gamma;\mathrm{D}}\psi)$ and, so by the nuclear theorem (Theorem V.12) there is a distribution $G_{\Gamma;\mathrm{D}}(x, y)$, called the **Dirichlet Green's function** so that

$$(\varphi, R_{\Gamma;\mathrm{D}}\psi) = \int \bar{\varphi}(x)\psi(y)G_{\Gamma;\mathrm{D}}(x, y)\, dx\, dy$$

for $\varphi, \psi \in \mathscr{S}$. The **Neumann Green's function** $G_{\Gamma;\mathrm{N}}(x, y)$ and **free Green's function** $G_0(x, y)$ are defined similarly. Of course,

$$G_0(x, y) = (4\pi)^{-1}|x - y|^{-1}e^{-|x-y|}$$

Lemma 4 Let B be an open ball containing Γ. Then $G_{\Gamma;\mathrm{D}} - G_0$ and $G_{\Gamma;\mathrm{N}} - G_0$ are C^∞ on $(\mathbb{R}^3\backslash\bar{B}) \times (\mathbb{R}^3\backslash\bar{B})$ and obey the estimates

$$|(G_{\Gamma;\mathrm{N}} - G_0)(x, y)| \le Ce^{-\frac{1}{2}|x| - \frac{1}{2}|y|} \tag{206a}$$

$$|(G_{\Gamma;\mathrm{D}} - G_0)(x, y)| \le Ce^{-\frac{1}{2}|x| - \frac{1}{2}|y|} \tag{206b}$$

In particular, if χ is the characteristic function of B, then

$$(1 + x^2)(1 - \chi)(R_0 - R_{\Gamma;\mathrm{D}})(1 - \chi)(1 + x^2)$$

and

$$(1 + x^2)(1 - \chi)(R_{\Gamma;\mathrm{N}} - R_0)(1 - \chi)(1 + x^2)$$

are Hilbert–Schmidt operators.

Proof We consider the Neumann case; the Dirichlet case is similar. Let $h, g \in C_0^\infty(\mathbb{R}^3\backslash\Gamma)$. Then $(H_{\Gamma;\mathrm{N}} + 1)h = (-\Delta + 1)h$ so that

$$\iint \overline{[(-\Delta + 1)h](x)}\, G_{\Gamma;\mathrm{N}}(x, y)g(y)\, dx\, dy = \int \overline{h(x)}\, g(x)\, dx$$

Therefore, as a distribution on $C_0^\infty((\mathbb{R}^3\backslash\Gamma) \times (\mathbb{R}^3\backslash\Gamma))$,

$$(-\Delta_x + 1)G_{\Gamma;\mathrm{N}}(x, y) = \delta(x - y)$$

so that

$$(-\Delta_x - \Delta_y + 2)(G_{\Gamma;\mathrm{N}}(x, y) - G_0(x, y)) = 0$$

It follows by elliptic regularity (Theorem IX.25) that $Q(x, y) \equiv G_{\Gamma;\mathrm{N}}(x, y) - G_0(x, y)$ is C^∞ on $(\mathbb{R}^3\backslash\Gamma) \times (\mathbb{R}^3\backslash\Gamma)$ and, in particular, on $(\mathbb{R}^3\backslash\bar{B}) \times (\mathbb{R}^3\backslash\bar{B})$. We first claim that for $x, y \in \mathbb{R}^3\backslash\bar{B}$,

$$Q(x, y) = \int_{z \in \partial B} \left[\frac{Q(z, y)}{\partial n_z} G_0(z, x) - Q(z, y) \frac{\partial G_0}{\partial n_z}(z, x)\right] d\Omega_z \qquad (207)$$

where $d\Omega$ is the surface measure on ∂B and n_z is the normal to B pointing outward from B at z.

Let $\tilde{B}$ be a sphere of very large radius enclosing ∂B, x, and y. Then (207) with $\int_{z \in \partial B}$ replaced by $\int_{z \in \partial B} - \int_{z \in \partial \tilde{B}}$ follows from $(-\Delta_x + 1)Q(x, y) = 0$ and $(-\Delta_x + 1)G_0(x, y) = \delta(x - y)$ by a standard argument using Green's formula

$$\int_\Omega (h\,\Delta g - g\,\Delta h)\,dx = \int_{\partial\Omega} (h\,\partial g/\partial n - g\,\partial h/\partial n)\,d\sigma$$

Thus (207) follows if we can show that the $\partial\tilde{B}$ integral goes to zero as $\partial\tilde{B}$ goes to ∞. Actually, we need only prove a weaker statement, namely, suppose we can prove that the $\partial\tilde{B}$ integral goes to zero as $r_0 \to \infty$ after we integrate over y with some $h \in C_0^\infty$ and integrate the radius of $\partial\tilde{B}$ from r_0 to $r_0 + 1$. Then by integrating the Green's formula result over the radius of $\partial\tilde{B}$ and taking $r_0 \to \infty$, we obtain (207) with y smeared out. We can then take h to a δ-function and obtain (207).

In the integral over the radius of $\partial\tilde{B}$, we can integrate the $\partial Q/\partial n_z$ by parts and so obtain an error term involving only G_0, $\partial G_0/\partial n_z$, and Q (no $\partial Q/\partial n_z$). Since G_0 and $\partial G_0/\partial n$ have exponential falloff as $|x - z| \to \infty$, it is sufficient to prove that $\int Q(z, y)h(y)\,dy$ is bounded as $z \to \infty$. But this follows from Lemma 1c! As a result, (207) holds for ∂B the boundary of any ball containing Γ.

Choose balls B_1 and B_2 with $\Gamma \subset B_1$, $\bar{B}_1 \subset B_2$, $\bar{B}_2 \subset B$. Now, since Q is C^∞ on $(\mathbb{R}^n\backslash\Gamma) \times (\mathbb{R}^n\backslash\Gamma)$, it follows that Q, $\nabla_x Q$, $\nabla_y Q$, and $\nabla_x \nabla_y Q$ are uniformly bounded on $\bar{B}_2\backslash B_1$ and, so by (207) with B replaced by B_1, Q and $\nabla_y Q$ are uniformly bounded for $x \in \mathbb{R}^3\backslash B$ and $y \in B_2$. By the symmetry of Q, we have that Q and $\nabla_x Q$ are uniformly bounded for $x \in B_2$ and $y \in \mathbb{R}^3\backslash B$. Using (207) with B replaced by B_2, this uniform bound, the exponential falloff of G_0, and the symmetry of Q, we obtain (206). ∎

Proof of Theorem XI.79 Since $0 \le R_0 - R_{\Gamma;\mathrm{D}} \le R_0$ by Lemma 1a, it suffices to prove that $\chi R_0 \chi$ is Hilbert–Schmidt to conclude that

$\chi(R_0 - R_{\Gamma;\mathrm{D}})\chi \in \mathcal{I}_2$ and thereby complete the proof by Lemmas 3 and 4. But $\chi R_0 \chi \in \mathcal{I}_2$ by direct calculation from the formula for G_0 or by Theorem XI.21. ▌

Proof of Theorem XI.80 By Lemma 1a,

$$0 \le R_{\Gamma;\mathrm{N}} - R_0 \le R_{\Gamma;\mathrm{N}} \le R_{\Gamma \cup \partial B;\mathrm{N}}$$

and by Lemma 1b, $\chi R_{\partial B \cup \Gamma;\mathrm{N}}\chi = \tilde{R}_{\partial B \cup \Gamma;\mathrm{N}} \oplus 0$ which is Hilbert–Schmidt by hypothesis. The theorem now follows from Lemmas 3 and 4. ▌

We now sketch a proof of Theorem XI.81 in a special case, leaving the details to the reader:

Lemma 5 Let $\Omega \subset B \subset \mathbb{R}^3$ be open balls with center 0. Let $\Gamma = \partial\Omega$, $S = \partial B$. Then $\tilde{R}_{\Gamma \cup S;\mathrm{N}}$, the operator on $L^2(B)$ with Neumann boundary conditions on Γ and S, is Hilbert–Schmidt.

Proof By Lemma 1b, $\tilde{R}_{\Gamma \cup S;\mathrm{N}} = R_1 \oplus R_2$ under the decomposition $L^2(B) = L^2(\Omega) \oplus L^2(B\backslash\Omega)$. We consider the R_1 case; the R_2 case is similar. $\tilde{H}_{\Gamma;\mathrm{N}}$ is a direct sum $\oplus_{\ell,m} \tilde{h}_{\ell,m}$ of operators under the decomposition $L^2(B) = \oplus \tilde{\mathscr{H}}_{\ell,m}$ where $\tilde{\mathscr{H}}_{\ell m} = \{\psi(r)Y_{\ell m}(\theta,\varphi)\}$. Under the isomorphism $\psi(r)Y_{\ell m} \leftrightarrow r\psi \equiv f$, $\tilde{\mathscr{H}}_{\ell m}$ goes over to $L^2(0, a)$ where $a = \mathrm{rad}(\Omega)$, and $\tilde{h}_{\ell m}$ to

$$h_{\ell m} = -d^2/dr^2 + \ell(\ell+1)r^{-2}$$

with boundary conditions

$$f(0) = 0, \qquad a^2(r^{-1}f)'(a) = af'(a) - f(a) = 0$$

One can therefore find explicitly the eigenfunctions of $h_{0,0}$ in terms of trigonometric functions and find that the nth eigenvalue obeys $E_{n,\ell=0} \ge C_1 n^2$. Since $h_{\ell m} \ge h_{0,0} + \ell(\ell+1)a^{-2}$, $E_{n,\ell} \ge C(n^2 + \ell^2)$, so

$$\sum_{n=0}^{\infty} (E_{n,\ell} + 1)^{-2} \le d_1 \int_0^{\infty} (x^2 + \ell^2 + 1)^{-2}\, dx = d(\ell^2 + 1)^{-3/2}$$

Thus

$$\mathrm{Tr}(R_1^2) = \sum_{\ell=0}^{\infty} (2\ell+1) \sum_{n=0}^{\infty} (E_{n,\ell} + 1)^{-2} < \infty \quad ▌$$

Lemma 6 Let Γ_1 and Γ_2 be two closed sets of measure zero respectively inside bounded open sets Ω_1, Ω_2 in $\mathbb{R}^3$. Let $S_i = \partial\Omega_i$. Suppose that there exists a C^∞ diffeomorphism F of a neighborhood of $\bar{\Omega}_1$ to a neighborhood of $\bar{\Omega}_2$ so that $F[\Omega_1] = \Omega_2$ and $F[\Gamma_1] = \Gamma_2$. Then $\tilde{R}_{\Gamma_1 \cup S_1; \mathrm{N}}$ is Hilbert–Schmidt if and only if $\tilde{R}_{\Gamma_2 \cup S_2; \mathrm{N}}$ is Hilbert–Schmidt.

Proof Consider the unitary map $U\colon L^2(\Omega_2, d^3x) \to L^2(\Omega_1, d^3x)$ given by

$$(Uf)(x) = (G^{1/2}f)(Fx)$$

where $G = \det\{J_{ij}\}$ and $J_{ij} = \{\partial F_i(x)/\partial x_j\}$. Then

$$U\tilde{H}_{\Gamma_2 \cup S_2; \mathrm{N}} U^{-1} = H'$$

where H' has the same form domain as $\tilde{H}_{\Gamma_1 \cup S_1; \mathrm{N}}$ and

$$\begin{aligned}(f, H'f) &= \int_{\Omega_1} \sum_i \left| \sum_j (J^{-1})_{ij} \frac{\partial(G^{1/2}f)}{\partial x_j} \right|^2 d^3x \\ &\le C_1 \int_{\Omega_1} \sum_i \left| \frac{\partial f}{\partial x_i} \right|^2 + |f|^2 \, d^3x \\ &= C_1(f, (H_{\Gamma_1 \cup S_1; \mathrm{N}} + 1)f)\end{aligned}$$

It follows that (Problem 117)

$$\tilde{R}_{\Gamma_1 \cup S_1; \mathrm{N}} \le C_2(H' + 1)^{-1}$$

so that $\tilde{R}_{\Gamma_1 \cup S_1; \mathrm{N}}$ is Hilbert–Schmidt if $(H' + 1)^{-1}$ is Hilbert–Schmidt. Since H' is unitarily equivalent to $\tilde{H}_{\Gamma_2 \cup S_2; \mathrm{N}}$, we see that $\tilde{R}_{\Gamma_1 \cup S_1; \mathrm{N}} \in \mathscr{I}_2$ if $\tilde{R}_{\Gamma_2 \cup S_2; \mathrm{N}} \in \mathscr{I}_2$. By symmetry, we can go in the other direction. ▮

Definition An open set Ω in $\mathbb{R}^3$ is called **starlike about x_0** in Ω if for any unit vector n, $\Omega \cap \{x_0 + tn \mid t \in [0, \infty)\} = \{x_0 + tn \mid t \in [0, a_n)\}$ for some $a_n > 0$. If a_n is a C^∞ function of n, we say that Ω has a **smooth boundary**.

Lemma 7 Let Γ_1 be the boundary of an open set D_1 that is starlike with smooth boundary with respect to x_0. Let

$$\Omega_1 = \{y \mid x_0 + (1 + \varepsilon)^{-1}(y - x_0) \in D_1\}$$

for some fixed $\varepsilon > 0$. Then, there is a C^∞ diffeomorphism F of a neighborhood of $\bar{\Omega}_1 \supset D_1$ onto a neighborhood of a ball $\bar{\Omega}_2$ such that $F[\Omega_1] = \Omega_2$ and such that $\Gamma_2 \equiv F[\Gamma_1]$ is the boundary of a sphere in Ω_2 with the same center as Ω_2. In particular, $\tilde{R}_{\Gamma_1 \cup S_1; \mathrm{N}}$ is Hilbert–Schmidt.

Proof Just define $F(x) = (x - x_0)a_{n(x)}^{-1}$ where $n(x) = (x - x_0)|x - x_0|^{-1}$. ▮

Finally, we can prove a special case of Theorem XI.81.

Theorem XI.81′ Let Γ be the union of a finite number of disjoint sets $\{\Gamma_j\}_{j=1}^k$ each of which is the smooth boundary of a bounded open starlike set Ω_j. Let B be any open ball containing Γ and let $S = \partial B$. Then $\tilde{R}_{\Gamma \cup S; N}$ is Hilbert–Schmidt.

Proof Let x_j be the point about which Ω_j is starlike. Let S_j be Γ_j scaled outward slightly from x_j. This can be done so that the S_j are disjoint and contained inside B. Let S' be the surface of a sphere concentric to S, inside S, and containing all the S_i (see Figure XI.13). Let $\chi_1, \ldots, \chi_k$ be the characteristic functions of the regions surrounded by the $S_j, j = 1, \ldots, k$. Let χ_{k+1} be the characteristic function of the shell between S and S' and let χ_0 be the characteristic function of the rest of B so that $\sum_{j=0}^{k+1} \chi_j \equiv 1$ on B. Then, by an extension of Lemma 3, it suffices to prove that $\chi_j R_{\Gamma \cup S; N} \chi_j$ is Hilbert–Schmidt for each $j = 0, 1, \ldots, k+1$. The case $j = 0$ is trivial since $G_{\Gamma \cup S; N}(x, y) - G_0(x, y)$ is C^∞ on $\overline{\operatorname{supp} \chi_0} \times \overline{\operatorname{supp} \chi_0}$ by Lemma 4 and $\chi_0(x) G_0(x, y) \chi_0(y)$ is the kernel of a Hilbert–Schmidt operator. For $j = 1, \ldots, k$,

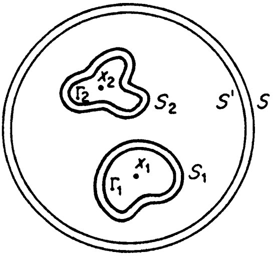


FIGURE XI.13 The sets S_i and S.

$$\chi_j \tilde{R}_{\Gamma \cup S; N} \chi_j \leq \chi_j \tilde{R}_{\Gamma \cup S_j \cup S; N} \chi_j = \tilde{R}_{\Gamma_j \cup S_j; N} \oplus 0$$

by Lemmas 1a and 1b. By Lemma 7, $\tilde{R}_{\Gamma_j \cup S_j; N}$ is Hilbert–Schmidt so $\chi_j \tilde{R}_{\Gamma \cup S; N} \chi_j$ is Hilbert–Schmidt too. The case $j = k+1$ is similar. ∎

XI.11 Optical and acoustical scattering II: The Lax–Phillips method

In this section we study a different approach to scattering theory developed by Lax and Phillips—different in that the main objects of study are certain families of subspaces of the Hilbert space of the interacting dynamics. As we shall see, this approach applies most naturally to classical wave equations that obey Huygens' principle rather than to quantum mechanics where the wave equations are dispersive and have infinite propagation speed. Nevertheless, by using the principle of invariance of the wave operators, it can also be applied in some quantum-mechanical situations (see Example 5).

The most beautiful and important aspect of the Lax–Phillips approach is that certain analyticity properties of the scattering operator arise naturally. When the interacting group satisfies the basic hypotheses of the theory, then there is a unitary map from $\mathscr{H}$ to $L^2(\mathbb{R}; N)$ where N is an auxiliary Hilbert space. In this representation of $\mathscr{H}$, the scattering operator acts by multiplication by an $\mathscr{L}(N)$-valued function $s(\sigma)$ which is unitary a.e. and which is the boundary value of an analytic $\mathscr{L}(N)$-valued function $s(z)$ in the upper half-plane. Typically, $s(z)$ can be meromorphically continued to the lower half-plane, and its poles are closely tied to the geometry and to the physical interpretation of the theory. We have already had examples of such continuations in Sections 7 and 8 and the appendix to Section 6.

A complete exposition of the Lax–Phillips theory is beyond the scope of this section. What we wish to do is to prove several of the basic theorems so that the underlying structure and the origin of the above-mentioned analyticity are clear. We then sketch several examples to show how the hypotheses are proven in practice. Detailed expositions and many applications can be found in the references discussed in the Notes.

The basic idea which is isolated and developed in the Lax–Phillips theory is that of incoming and outgoing subspaces.

Definition Let $U(t)$ be a strongly continuous unitary group on a Hilbert space $\mathscr{H}$. A closed subspace $D_+ \subset \mathscr{H}$ is said to be **outgoing** if:

(i) $U(t)[D_+] \subset D_+$ for $t \geq 0$.
(ii) $\bigcap_t U(t)[D_+] = \{0\}$.
(iii) $\overline{\bigcup_t U(t)[D_+]} = \mathscr{H}$.

Similarly, if D_- satisfies (ii), (iii) and

(i′) $U(t)[D_-] \subset D_-$ for $t \leq 0$,

then D_- is said to be **incoming**.

This terminology arose naturally in applications. For instance, in the Hilbert space for the free wave equation on $\mathbb{R}^3$ (see Example 1), D_+ is just the set of initial data so that the solution $u(x, t)$ vanishes if $|x| \leq t$; that is, physically, the waves are going out in the future. Similarly, D_- is the set of initial data so that $u(x, t)$ vanishes if $|x| \leq -t$. Such a solution is coming in in the past.

An example of an outgoing subspace can be constructed as follows. Let N be a Hilbert space, let $\mathscr{H} = L^2(\mathbb{R}; N)$, and define $U(t)$ to be translation to the right by t units, that is, $(U(t)f)(s) = f(s - t)$. Then

$$D_+ = L^2(0, \infty; N) \equiv \{f \in L^2(\mathbb{R}; N) \mid f(s) = 0 \text{ for } s < 0\}$$

is outgoing. The main structure theorem of this section says that in fact all outgoing subspaces are essentially of this form.

Theorem XI.82 Let $U(t)$ be a strongly continuous unitary group on a Hilbert space $\mathscr{H}$ and let D_+ be an outgoing subspace for $U(t)$. Then there is an auxiliary Hilbert space N and a unitary map $\mathscr{R}_+$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}_+[D_+] = L^2(0, \infty; N)$ and $U_+(t) \equiv \mathscr{R}_+ U(t)\mathscr{R}_+^{-1}$ is translation to the right by t units. Similarly, if D_- is an incoming subspace, there is a unitary map $\mathscr{R}_-$ onto $L^2(\mathbb{R}; N')$ so that $\mathscr{R}_-[D_-] = L^2(-\infty, 0; N')$ and $U_-(t) \equiv \mathscr{R}_- U(t)\mathscr{R}_-^{-1}$ is translation to the right by t units. If $U(t)$ has both incoming and outgoing subspaces, N and N' can be chosen to be the same, although $\mathscr{R}_+$ may not equal $\mathscr{R}_-$. These representations are unique up to isomorphisms of N.

$U_+(t)$, $L^2(0, \infty; N)$, and $L^2(\mathbb{R}; N)$ are said to be an **outgoing translation representation** of $U(t)$, D_+, and $\mathscr{H}$. Similarly, $U_-(t)$, $L^2(-\infty, 0; N)$, and $L^2(\mathbb{R}; N)$ are said to be an **incoming translation representation** of $U(t)$, D_-, and $\mathscr{H}$.

Before proving the theorem, we make several remarks. First, if $U(t)$ has incoming and outgoing subspaces, we can construct a scattering operator as follows. For $\varphi \in \mathscr{H}$, let $\varphi_- = \mathscr{R}_- \varphi$ and $\varphi_+ = \mathscr{R}_+ \varphi$, and define $\tilde{S}$ to be the map $\tilde{S}: \varphi_- \mapsto \varphi_+$, that is,

$$\tilde{S} = \mathscr{R}_+ \mathscr{R}_-^{-1}$$

$\tilde{S}$ is a unitary map from $L^2(\mathbb{R}; N)$ to itself. S is defined by pulling this operator back to $\mathscr{H}$:

$$S \equiv \mathscr{R}_-^{-1}(\mathscr{R}_+ \mathscr{R}_-^{-1})\mathscr{R}_- = \mathscr{R}_-^{-1}\mathscr{R}_+$$

Finally, letting $\mathscr{F}$ denote the Fourier transform, a unitary map from $L^2(\mathbb{R}; N)$ to itself, we define

$$\hat{S} \equiv \mathscr{F}\tilde{S}\mathscr{F}^{-1}$$

S, $\hat{S}$, and $\tilde{S}$ are clearly unitarily equivalent, so we shall call them all **the scattering operator**, distinguishing between the representations by the ˆ and ˜.

Since $\mathcal{R}_\pm U(t) = U_\pm(t)\mathcal{R}_\pm$ and $U_+(t) = U_-(t)$, S commutes with $U(t)$. Since $\tilde{S}$ commutes with translation, it should intuitively be given by convolution by an $\mathcal{L}(N)$-valued function τ on $\mathbb{R}$, so $\hat{S}$ should be given by multiplication by an operator-valued function $s = (2\pi)^{1/2}\hat{\tau}$. If we have the additional hypothesis that $D_- \subset D_+^\perp$, then $\tilde{S}$ takes $L^2(-\infty, 0; N)$ into itself, which requires that τ have support on $(-\infty, 0]$. The Paley–Wiener theorem thus suggests that s should have an analytic extension to the upper half-plane. This is the source of the analyticity described in the introductory remarks above (details are given in Theorem XI.89 and its corollary).

Notice that the definition of the scattering operator did not mention any "free dynamics." In practice, the incoming and outgoing subspaces are constructed by using the free dynamics; and $\mathcal{R}_+$ and $\mathcal{R}_-$ turn out to be (unitarily equivalent to) the usual wave operators. This is further discussed below. However, the construction above raises the possibility of defining S when there is no "natural" candidate for the free dynamics or in situations where the convergence of interacting solutions to free solutions as $t \to \pm\infty$ is too slow to allow the usual construction of the wave operators. However, we emphasize that the construction does depend on more than the interacting dynamics $U(t)$. For example, once one has an outgoing translation representation of $\mathcal{H}$ as $L^2(-\infty, \infty; N)$, one can take $\tilde{D}_- = \mathcal{R}_+^{-1}[L^2(-\infty, 0; N)]$. For the pair D_+, $\tilde{D}_-$, the S-matrix is I. Typically, the additional structure that determines the choice of D_+ and D_- is some underlying geometry.

One inherent restriction of the theory as it stands is apparent from Theorem XI.82 itself. The existence of an incoming or outgoing translation representation for $U(t)$ implies that its generator H has purely absolutely continuous spectrum on the whole real axis and that the spectrum has uniform multiplicity. This, however, does not make applications to quantum mechanics impossible (see Example 5).

As motivation for our proof of Theorem XI.82, we first prove the discrete analogue.

Theorem XI.83 Let V be a unitary operator on a separable Hilbert space $\mathcal{H}$. Let D_+ be a closed subspace of $\mathcal{H}$ so that:

(i) $V[D_+] \subset D_+$.
(ii) $\bigcap_{k \in \mathbb{Z}} V^k[D_+] = \{0\}$.
(iii) $\overline{\bigcup_{k \in \mathbb{Z}} V^k[D_+]} = \mathcal{H}$.

Then there is a Hilbert space N and a unitary map $\imath_+$ of $\mathcal{H}$ onto $\ell_2(-\infty, \infty; N)$ such that

$$\imath_+[D_+] = \{f \mid f(n) = 0,\ n < 0\} \equiv \ell_2[0, \infty; N)$$

and $\tilde{V} = \imath_+ V \imath_+^{-1}$ is the right shift. This representation is unique up to isomorphism of N.

Proof We prove the existence of $\imath_+$ and leave uniqueness to the reader (Problem 121). Let $N = D_+ \cap (V[D_+])^\perp$ which is a closed subspace of $\mathscr{H}$. Since V is unitary,

$$VN = VD_+ \cap V^2 D_+^\perp \subset VD_+ \subset N^\perp$$

so we can form the direct sum $N \oplus VN$. Since $N \oplus VD_+ = D_+$, we have $VN \oplus V^2 D_+ = VD_+$ so that

$$N \oplus VN \oplus V^2 D_+ = D_+$$

or equivalently,

$$N \oplus VN = D_+ \cap V^2 D_+^\perp$$

In the same way one sees inductively that

$$V^j N \subset V^j D_+ \subset (N \oplus \cdots \oplus V^{j-1} N)^\perp$$

$$N \oplus \cdots \oplus V^j N = D_+ \cap V^{j+1} D_+^\perp \tag{208}$$

By (i), $D_+ \supseteq VD_+ \supseteq \cdots \supseteq V^j D_+$ so by (ii) and (208):

$$\bigoplus_{k \geq 0} V^k N = D_+ \tag{209}$$

Applying V^{-1} to $N \oplus VD_+ = D_+$, we see that

$$V^{-1} N \oplus D_+ = V^{-1} D_+$$

so that inductively one sees that

$$\bigoplus_{k \geq \ell} V^k N = V^\ell D_+$$

for ℓ any integer, positive or negative. Taking $\ell \to -\infty$ and using (iii), we see that

$$\bigoplus_{k \in \mathbb{Z}} V^k N = \mathscr{H}$$

Thus any $\varphi \in \mathscr{H}$ can be uniquely written

$$\varphi = \sum_k V^k \varphi_k, \qquad \varphi_k \in N$$

with $\|\varphi\|^2 = \sum_k \|\varphi_k\|^2$. As a result, the map

$$\varphi \xmapsto{\imath_+} \{\varphi_k\}_{k=-\infty}^{\infty}$$

is a unitary map of $\mathscr{H}$ onto $\ell_2(-\infty, \infty; N)$. By (209), $\imath_+ D_+ = \ell_2[0, \infty; N)$, and it is easy to check that $\tilde{V}$ is the right shift. ▮

There are at least three fairly distinct proofs of Theorem XI.82. One reverses the analysis of Theorem XI.84 below and uses von Neumann's uniqueness theorem to prove Theorem XI.82. The second uses techniques of Fourier analysis, Theorem XI.83, and the Cayley transform. The proof we give depends on spectral multiplicity theory (see Section VII.2) and has its roots in general group theoretic methods, especially Mackey's imprimitivity theorem. We recall that two measures are called **equivalent** if and only if they are mutually absolutely continuous. The key technical result we need in our proof of Theorem XI.82 is closely connected to the fact that Lebesgue measure is the unique translation invariant measure on $\mathbb{R}$ (Problem 122).

Lemma Suppose that $d\mu$ is a nontrivial Borel measure on $\mathbb{R}$ with the property that $d\mu(\cdot + a)$ is equivalent to $d\mu$ for all $a \in \mathbb{R}$. Then $d\mu$ is equivalent to Lebesgue measure.

Proof By hypothesis

$$d\mu(x + y) = g_y(x)\, d\mu(x) \tag{210}$$

It is immediate that $g_y(x)$ is measurable in x for each fixed y and $\int h(x) g_y(x)\, d\mu(x) = \int h(x - y)\, d\mu(x)$ is measurable in y for each measurable h, and thus $g_y(x)$ is jointly measurable.

Fix $h \geq 0$ with $\int h(y)\, dy = 1$ and let f be a simple function. Then, freely using Fubini's theorem:

$$\begin{aligned} \alpha \equiv \int f(x)\, d\mu(x) &= \iint f(x) h(y)\, d\mu(x)\, dy \\ &= \iint f(x + y) g_y(x) h(y)\, d\mu(x)\, dy \end{aligned} \tag{211}$$

by (210). Make the change of variables $z = x + y$ for fixed x, so that

$$\int f(x + y) g_y(x) h(y)\, dy = \int f(z) g_{z-x}(x) h(z - x)\, dz$$

by the translation invariance of Lebesgue measure. Thus

$$\alpha = \int f(z) G(z)\, dz$$

where

$$G(z) = \int g_{z-x}(x)h(x-z)\,d\mu(x)$$

Since f is arbitrary,

$$d\mu(x) = G(x)\,dx$$

Now, fix $h \geq 0$ with $\int h(y)\,d\mu(y) = 1$ and compute, as above, that

$$\begin{aligned}\int f(x)\,dx &= \iint f(x)h(y)\,d\mu(y)\,dx\\ &= \iint f(x+y)h(y)\,dx\,d\mu(y)\\ &= \iint f(z)h(z-x)g_{-x}(z)\,d\mu(z)\,dx\\ &= \int f(z)H(z)\,d\mu(z)\end{aligned}$$

with $H(z) = \int h(z-x)g_{-x}(z)\,dx$. Thus

$$dx = H(x)\,d\mu(x) \blacksquare$$

Proof of Theorem XI.82 Motivated by the proof of Theorem XI.83, we define

$$D_+(t) \equiv U(t)[D_+], \qquad t \in \mathbb{R}$$

$$D_+(\infty) \equiv \{0\}, \qquad D_+(-\infty) \equiv \mathscr{H}$$

and for $a < b$ we define

$$N(a, b] = D_+(a) \cap D_+(b)^{\perp}$$

Let $P_{(a,b]}$ be the orthogonal projection onto $N(a, b]$. Then from properties (i)–(iii) of D_+ and the fact that $U(t)$ is continuous, it is easy to check that $\{P_{(a,b]}\}$ generates a projection-valued measure $\{P_\Omega\}$ that satisfies $U(t)P_\Omega U(-t) = P_{\Omega+t}$. Introducing the operator

$$X = \int_{\mathbb{R}} \lambda\,dP_\lambda$$

this implies that $U(t)XU(t)^{-1} = X + t$. It follows from the uniqueness of the spectral multiplicity measure classes (Theorem VII.6) that the spectral measure classes of X are invariant under translation. Thus, by the lemma, each class must be the one containing Lebesgue measure. Since the measure classes are disjoint, there is only one measure class, that is, X is a self-adjoint operator of uniform multiplicity m for some m with corresponding measure dx. It follows that there is a Hilbert space N of dimension m and a unitary map $\mathscr{Q}_+ : \mathscr{H} \to L^2(\mathbb{R}, dx; N)$ so that $\mathscr{Q}_+ P_\Omega \mathscr{Q}_+^{-1}$ is multiplication by χ_Ω, the characteristic function of Ω.

Let $W(t) = \mathscr{Q}_+ U(t)\mathscr{Q}_+^{-1}$ and let $T_0(t)$ be translation to the right by t units on $L^2(\mathbb{R}, dx; N)$. Then, for each t, $W(t)T_0(t)^{-1}$ commutes with each P_Ω; so by Theorem XIII.84, there is an $\mathscr{L}(N)$-valued measurable function $K_t(s)$ such that

$$(W(t)T_0(-t)f)(s) = K_t(s)f(s)$$

$K_t(s)$ is defined only almost everywhere in s, but for definiteness we make a choice for all s. Then

$$(W(t)f)(s) = K_t(s)f(t+s)$$

The group property $W(t)W(u) = W(t+u)$ implies that

$$K_t(s)K_u(t+s) = K_{t+u}(s) \tag{212}$$

(212) holds in the following sense: For each t and u, it holds for almost all s. Thus it holds for almost all triples $\langle s, t, u\rangle$, so we can choose a fixed value of s so that (212) holds for almost all $\langle t, u\rangle$. For that fixed value of s, define

$$(Bf)(t) = K_{t-s}(s)f(t)$$

Then

$$\begin{aligned}(BW(a)B^{-1}f)(t) &= K_{t-s}(s)K_a(t)[K_{t+a-s}(s)]^{-1}f(t+a)\\ &= f(t+a)\end{aligned}$$

for almost all t and a where we have used (212) with the change of variables $t' = t+s$, $u' = a$. It follows that $BW(a)B^{-1} = T_0(a)$ for almost all a, and so by continuity for all a. Letting $\mathscr{R}_+ = B\mathscr{Q}_+$, the theorem results. ∎

Theorem XI.82 can be used to provide a proof of von Neumann's theorem (Theorem VIII.14) on the uniqueness of representations of the canonical commutation relations.

Theorem XI.84 (von Neumann's theorem) Let $U(t)$ and $V(s)$ be two strongly continuous one-parameter groups on a Hilbert space $\mathscr{H}$ that satisfy

$$U(t)V(s) = e^{its}V(s)U(t) \qquad \text{all } t \text{ and } s$$

Then there is a Hilbert space N and a unitary map $\mathscr{R}$ from $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}U(t)\mathscr{R}^{-1}$ is translation to the right by t units and $\mathscr{R}V(s)\mathscr{R}$ is multiplication by $e^{-i\lambda s}$.

Proof Let P and Q be the self-adjoint operators with $U(t) = e^{-itP}$ and $V(s) = e^{-isQ}$. Let $\mathscr{D}$ denote the set of vectors in $\mathscr{H}$ of the form

$$\varphi_f = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(t, s)U(t)V(s)\varphi \, dt \, ds$$

where $\varphi \in \mathscr{H}$ and $f \in C_0^\infty(\mathbb{R}^2)$. Exactly as in the proof of Theorem VIII.8, one easily shows that $\mathscr{D}$ is dense in $\mathscr{H}$, $\mathscr{D} \subset D(Q)$, $\mathscr{D} \subset D(P)$, and that $\mathscr{D}$ is invariant under $U(s)$ and $V(t)$. By Theorem VIII.10, P and Q are essentially self-adjoint on $\mathscr{D}$. Let $\psi \in \mathscr{D}$, then since $U(t)\psi$ is in $\mathscr{D}$ also, we may differentiate both sides of the equality

$$U(t)V(s)\psi = e^{its}V(s)U(t)\psi$$

with respect to s. Setting $s = 0$, we obtain

$$U(t)QU(-t)\psi = (Q - tI)\psi \tag{213}$$

Since this relation is true on $\mathscr{D}$, which is a core for Q and $Q - tI$, we conclude that Q and $Q - tI$ are unitarily equivalent and (213) holds for all $\psi \in D(Q)$. Now, let $\{E_\Omega\}$ be the spectral family for Q. Then $\{U(t)E_\Omega U(-t)\}$ is the spectral family for $U(t)QU(-t)$. Since $E_\Omega = \chi_\Omega(Q)$, (213) implies that

$$U(t)E_{(-\infty,\lambda)}U(-t) = E_{(-\infty,\lambda+t)} \tag{214}$$

for all λ and t in $\mathbb{R}$.

Set $D_- = \text{Ran } E_{(-\infty,0]}$. We shall show that D_- is an incoming subspace for $U(t)$ on $\mathscr{H}$. First, (214) implies that $U(t)D_- = \text{Ran } E_{(-\infty,\lambda+t]}$ for all t. Thus:

(i) $U(t)D_- \subset D_-, t \le 0$;
(ii) $\bigcap_t U(t)D_- = \{0\}$;
(iii) $\overline{\bigcup_t U(t)D_-} = \mathscr{H}$;

by the usual properties of the spectral projections. So, by Theorem XI.82, there is an auxiliary Hilbert space N and a unitary map $\mathscr{R}_-$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $\mathscr{R}_- D_- = L^2(-\infty, 0; N)$ and $\mathscr{R}_- U(t)\mathscr{R}_-^{-1}$ is translation to the right by t units. Finally, since $\mathscr{R}_- E_{(-\infty,0)}\mathscr{R}_-^{-1} = \chi_{(-\infty,0)}$, (214) implies that $\mathscr{R}_- E_{(-\infty,\lambda)}\mathscr{R}_-^{-1} = \chi_{(-\infty,\lambda)}$ for all λ. Thus $\mathscr{R}_- Q\mathscr{R}_-^{-1}$ is multiplication by λ and $\mathscr{R}_- e^{-iQs}\mathscr{R}_-^{-1}$ equals multiplication by $e^{-i\lambda s}$. ∎

Theorem XI.82 can be reformulated using the Fourier transform. Defined by the usual formula, the Fourier transform $\mathscr{F}$ is a unitary map of $L^2(\mathbb{R}; N)$ onto itself. It takes $L^2(0, \infty; N)$ onto the Hardy–Lebesgue class $\mathscr{H}^2_-(\mathbb{R}; N)$ and $L^2(-\infty, 0; N)$ onto $\mathscr{H}^2_+$ (see the Notes to Section IX.3).

Theorem XI.85 Let D_+ be an outgoing subspace for the unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Then there is an auxiliary Hilbert space N and a unitary map $\mathscr{F} \circ \mathscr{R}_+$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ such that $\mathscr{F} \circ \mathscr{R}_+[D_+] = \mathscr{H}^2_-(\mathbb{R}; N)$ and $(\mathscr{F} \circ \mathscr{R}_+)U(t)(\mathscr{F} \circ \mathscr{R}_+)^{-1}$ is multiplication by $e^{-i\sigma t}$.

The above representation is called an **outgoing spectral representation** for $U(t)$, D_+, and $\mathscr{H}$. For an incoming subspace a similar theorem holds except that $\mathscr{F} \circ \mathscr{R}_+$ is replaced by $\mathscr{F} \circ \mathscr{R}_-$ and $\mathscr{H}^2_-(\mathbb{R}; N)$ is replaced by $\mathscr{H}^2_+(\mathbb{R}; N)$.

The discussion after the statement of Theorem XI.82 shows that if we have incoming and outgoing subspaces, then we can construct a scattering theory. But, Theorem XI.82 says nothing about how one actually constructs incoming and outgoing subspaces for $U(t)$. Since $U(t)$ is the dynamics of an interacting system, this is not a trivial question. In applications, the construction depends heavily on the fact that $U(t)$ is closely related to a free dynamics $U_0(t)$ and that $U_0(t)$ has many special properties. For example, let $W_0(t)$ and $W(t)$ be the unitary groups for acoustical waves in free space and in inhomogeneous media constructed in the preceding section. Suppose that the region of inhomogeneity is contained inside some finite ball $\mathscr{B}_{r_0}$. The Hilbert spaces on which $W_0(t)$ and $W(t)$ act are equivalent, and the norms are equal for pairs of functions whose support lies outside $\mathscr{B}_{r_0}$. Furthermore, any data of compact support will eventually be propagated outside of $\mathscr{B}_{r_0}$ by $W_0(t)$; and as long as the data stay away from $\mathscr{B}_{r_0}$, $W_0(t)$ and $W(t)$ agree. These and other special properties of $W_0(t)$ and $W(t)$ are exploited in Examples 1 and 2 below. For the moment, we return to the general setting and formulate precisely what we mean by a "close relationship" between $U(t)$ and $U_0(t)$.

Suppose that $U(t)$ and $U_0(t)$ are strongly continuous unitary groups on Hilbert spaces $\mathscr{H}$ and $\mathscr{H}_0$ and let J be an identification operator from $\mathscr{H}_0$ to $\mathscr{H}$. Suppose that:

(0) There exist subspaces $D^{r_0}_{\pm} \subset \mathscr{H}_0 \cap \mathscr{H}$ so that the $\mathscr{H}_0$-norm and the $\mathscr{H}$-norm are the same on $D^{r_0}_{\pm}$ and J is the identity on $D^{r_0}_{\pm}$.
(1) $D^{r_0}_{+}$ and $D^{r_0}_{-}$ are incoming and outgoing for $U(t)$ *and* for $U_0(t)$.
(2) $U(t)$ and $U_0(t)$ act the same on $D^{r_0}_{+}$ for $t \geq 0$. $U(t)$ and $U_0(t)$ act the same on $D^{r_0}_{-}$ for $t \leq 0$.

(3) There is a Hilbert space N and a unitary map $\varphi \xmapsto{\mathscr{R}_0} \tilde{\varphi}$ of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ so that $D_+^{r_0}$ and $D_-^{r_0}$ go over to $L^2(r_0, \infty; N)$ and $L^2(-\infty, -r_0; N)$, respectively, where r_0 is some positive number, and $U_0(t)$ goes over to translation by t. That is, up to a shift of r_0 units, this representation is both incoming *and* outgoing for $U_0(t)$.

Let $T_0(t)$ denote translation to the right on $L^2(\mathbb{R}; N)$. To construct an outgoing translation representation for $U(t)$, for each φ in $D_+^{r_0}$, we map $U(t)\varphi$ to $T_0(t)\tilde{\varphi}$. By (2), this map is well defined, it is norm preserving, and by (iii) it is densely defined. Further, it has dense range since $\mathscr{R}_0$ takes $D_+^{r_0}$ onto $L^2(r_0, \infty; N)$. The map thus extends to a unitary map of $\mathscr{H}$ onto $L^2(\mathbb{R}; N)$ under which $U(t)$ goes over to T_0 and $D_+^{r_0}$ goes to $L^2(r_0, \infty; N)$. Left shift by $T_0(-r_0)$ makes this an outgoing translation representation for $U(t)$. A similar construction creates an incoming translation representation. We denote the maps onto the incoming and outgoing translation representations by $\mathscr{R}_+$ and $\mathscr{R}_-$ as before. Notice that, by (3), $D_+^{r_0}$ and $D_-^{r_0}$ are orthogonal. This will have important consequences later.

In this situation, where we have a free group $U_0(t)$, it is natural to ask how the Lax–Phillips scattering operator is related to the usual wave operators and scattering operator. Let D be the dense set of vectors φ in $\mathscr{H}_0$ so that $\mathscr{R}_0 \varphi$ has compact support. If $\varphi \in D$, then for some s, $U_0(s)\varphi \in D_+^{r_0}$ so by (2), $U(-t)JU_0(t)\varphi$ is independent of t for $t \geq s$. Thus,

$$\Omega^- \varphi = \lim_{t \to \infty} U(-t)JU_0(t)\varphi$$

exists. Since D is dense, the limit exists on all of $\mathscr{H}_0$; a similar argument proves the existence of Ω^+.

Now, notice that if $\psi \in D_+^{r_0}$ then $\Omega^- \psi = \psi$; so if $\varphi \in D$ and $U_0(s_1)\varphi \in D_+^{r_0}$, then

$$\Omega^- U_0(s_1)\varphi = U_0(s_1)\varphi$$

Therefore,

$$\begin{aligned} \mathscr{R}_+ \Omega^- \varphi = T_0(-s_1)\mathscr{R}_+ \Omega^- U_0(s_1)\varphi &= T_0(-s_1)\mathscr{R}_+ U_0(s_1)\varphi \\ &= T_0(-r_0 - s_1)\mathscr{R}_0 U_0(s_1)\varphi \\ &= T_0(-r_0)\mathscr{R}_0 \varphi \end{aligned}$$

since $\mathscr{R}_+ = T_0(-r_0)\mathscr{R}_0$ on $D_+^{r_0}$. Since such φ are dense, we have

$$\mathscr{R}_+ \Omega^- = T_0(-r_0)\mathscr{R}_0$$

and similarly

$$\mathscr{R}_- \Omega^+ = T_0(r_0)\mathscr{R}_0$$

Since $\mathcal{R}_0$, $\mathcal{R}_\pm$, and $T_0(t)$ are unitary, this shows that Ran $\Omega^+ = \mathcal{H} =$ Ran Ω^-, so the wave operators are complete. Finally,

$$\begin{aligned}(\Omega^-)^{-1}\Omega^+ &= \mathcal{R}_0^{-1}T_0(r_0)\mathcal{R}_+\mathcal{R}_-^{-1}T_0(r_0)\mathcal{R}_0\\ &= \mathcal{R}_0^{-1}T_0(r_0)\tilde{S}T_0(r_0)\mathcal{R}_0\\ &= \mathcal{R}_0^{-1}(T_0(2r_0)\tilde{S})\mathcal{R}_0\end{aligned}$$

So, except for the inessential factor $T_0(2r_0)$, $(\Omega^-)^{-1}\Omega^+$ is just the Lax–Phillips scattering operator pulled back to $\mathcal{H}_0$. We summarize:

Theorem XI.86 Let $U_0(t)$, $U(t)$, and J satisfy the hypotheses (0)–(3) and let $\mathcal{R}_0$, T_0, and r_0 be defined as above. Then the wave operators $\Omega^\pm$ exist, are complete, and

$$(\Omega^-)^{-1}\Omega^+ = \mathcal{R}_0^{-1}(T_0(2r_0)\tilde{S})\mathcal{R}_0 \tag{215}$$

Example 1 (the free wave equation in three dimensions) We have already formulated the free wave equation as a Hilbert space problem in Sections X.13 and XI.10. We shall use the notation introduced in Section XI.10, setting $c_0 = 1$ by a suitable choice of units. For initial data $\varphi \in \mathcal{H}_0$, the first component $u(x, t) = (W_0(t)\varphi)_1$ satisfies the free wave equation (186) if φ is smooth enough. The primary fact that we need is Huygens' principle:

Theorem XI.87 (Huygens' principle) Let $W_0(t)$ be the unitary group for the free wave equation on $\mathbb{R}^3$ and set $u(x, t) = (W_0(t)\varphi)_1$. Suppose that $\varphi = \langle f, g\rangle \in \mathcal{H}$ has compact support. Then

$$\operatorname{supp} u(x, t) \subset \left\{x \,\middle|\, |x - y| = t \text{ for some } y \in \operatorname{supp}\langle f, g\rangle\right\}$$

Proof Suppose first that $f = 0$ and that $g \in C_0^\infty(\mathbb{R}^3)$. We shall derive an explicit formula for the solution of (186) in the case $c_0 = \rho_0 = 1$. In order to solve (186), we need just find a u so that $\hat{u}_{tt}(k, t) = -k^2\hat{u}(k, t)$, $\hat{u}(k, 0) = 0$, and $\hat{u}_t(k, 0) = \hat{g}(k)$. This is easily done by setting

$$\hat{u}(k, t) = \frac{\sin|k|t}{|k|}\hat{g}(k)$$

Let H be the tempered distribution whose Fourier transform is $|k|^{-1}\sin|k|t$. Then

$$\begin{aligned}u(x, t) &= \mathcal{F}^{-1}(|k|^{-1}\sin|k|t\,\hat{g}(k))\\ &= (2\pi)^{-3/2}H * g\end{aligned}$$

so in order to represent the solution we must just find H. Let dS_R denote the area measure on the sphere of radius R. dS_R is a tempered distribution and using θ for the angle between x and k,

$$\begin{aligned}\widehat{dS_R}(k) &= (2\pi)^{-3/2}\int e^{-ik\cdot x}\,dS_R(x)\\ &= (2\pi)^{-3/2}\int_0^\pi d\theta\int_0^{2\pi} e^{-i|k|R\cos\theta}R^2\sin\theta\,d\psi\\ &= (2\pi)^{-1/2}R^2\int_0^\pi e^{-i|k|R\cos\theta}\sin\theta\,d\theta\\ &= \frac{2R\sin|k|R}{(2\pi)^{1/2}|k|}\end{aligned}$$

Thus for $t > 0$, $H = (2t)^{-1}(2\pi)^{1/2}\,dS_t$ and

$$u(x, t) = \frac{1}{4\pi t}\int_{\mathbb{R}^3} g(x+y)\,dS_t(y)$$

A similar representation holds for $t < 0$. Notice that $v = u_t$ satisfies (186) too, along with the initial conditions $v(0, t) = g$, $v_t(0, t) = 0$. Thus, for $f, g \in C_0^\infty(\mathbb{R}^3)$, we can write the solution of (186) as

$$u(x, t) = \frac{1}{4\pi t}\int_{\mathbb{R}^3} g(x+y)\,dS_t(y) + \frac{d}{dt}\left(\frac{1}{4\pi t}\int_{\mathbb{R}^3} f(x+y)\,dS_t(y)\right) \tag{216a}$$

and from this representation Huygens' principle follows immediately for C_0^∞ data.

Now suppose that $\varphi = \langle f, g\rangle \in \mathscr{H}_0$ with support in a compact set K and let Σ_t be the set where $u(x, t)$ is supposed to be supported according to Huygens' principle. Let $K^{(\varepsilon)}$ and $\Sigma_t^{(\varepsilon)}$ be the sets K and Σ_t plus all the points a distance less than ε away. Then there is a sequence $\varphi_n = \langle f_n, g_n\rangle$ of pairs of C_0^∞ functions with support in $K^{(\varepsilon)}$ so that $\varphi_n \to \varphi$ in $\mathscr{H}_0$. Since $W_0(t)$ is unitary, $W_0(t)\varphi_n \to W_0(t)\varphi$ and, in particular,

$$\int_{\mathbb{R}^3} |\nabla(u_n - u)(x)|^2\,dx \to 0$$

By the uncertainty principle lemma (Section X.2),

$$\begin{aligned}\int_{|x|\le r} |u(x, t) - u_n(x, t)|^2\,dx &\le 4r^2\int_{\mathbb{R}^3}\frac{1}{4|x|^2}|u(x, t) - u_n(x, t)|^2\,dx\\ &\le 4r^2\int_{\mathbb{R}^3}|\nabla(u(x, t) - u_n(x, t))|^2\,dx \end{aligned}\tag{216b}$$

so that in each ball of radius r a subsequence of $\{u_n\}$ converges to u pointwise a.e. Thus u is zero outside $\Sigma^{(\varepsilon)}$ since each of the u_n is zero there. Since ε is arbitrary, u is supported in Σ_t. ▌

Corollary Suppose that $\operatorname{supp}\langle f, g\rangle$ is contained in the ball of radius r. Then

$$u(x, t) = 0 \qquad \text{for} \quad |x| > r + t \tag{217a}$$

$$u(x, t) = 0 \qquad \text{for} \quad |x| < |t| - r \tag{217b}$$

(217a) is an expression of the finite propagation speed and holds in all dimensions. (217b) is an expression of Huygens' principle which holds only in odd dimensions greater than or equal to three.

Now we define

$$D_+ = \{\varphi \in \mathscr{H}_0 \,|\, u(x, t) = (W_0(t)\varphi)_1 \text{ is zero for } |x| \le t,\ t > 0\}$$

$$D_- = \{\varphi \in \mathscr{H}_0 \,|\, u(x, t) = (W_0(t)\varphi)_1 \text{ is zero for } |x| \le -t,\ t < 0\}$$

To check that D_+ is an outgoing subspace we proceed as follows. D_+ is closed by the unitarity of $W_0(t)$ and the inequality (216b). To prove (i) notice that if $\varphi \in D_+$, then

$$(W_0(t)W_0(s)\varphi)_1 = (W_0(t+s)\varphi)_1 = u(x, t+s)$$

so $(W_0(t)W_0(s)\varphi)_1$ is zero if $t > 0$ and $|x| \le t + s$. Thus if $s \ge 0$, $W_0(s)\varphi \in D_+$. Secondly, suppose that $\psi \in \bigcap_s W_0(s)[D_+]$. Since $\varphi \in D_+$ implies that

$$\operatorname{supp}(W_0(s)\varphi)_1 \subset \mathbb{R}^3 \Big\backslash \Big\{x \,\Big|\, |x| \le s\Big\}$$

$\psi \in W_0(s)[D_+]$ for all $s > 0$ implies that $(\psi)_1 \equiv 0$. But for $\varphi \in D_+$, $(d/dt) \times (W_0(t)\varphi)_1 = (W_0(t)\varphi)_2$ so $(\psi)_2 \equiv 0$ too. Thus $\psi \equiv 0$, which proves (ii). Finally, notice that if $\operatorname{supp} \varphi \subset \{x \,|\, |x| \le R\}$, then by (217b), $W_0(R)\varphi \in D_+$. Thus, $\bigcup_t W_0(t)D_+$ contains all the C^∞ data of compact support, so (iii) holds. The proof that D_- is incoming is similar. Thus by Theorem XI.82 there exist incoming and outgoing translation representations for $W_0(t)$.

In practice one wants a translation representation that is both incoming *and* outgoing for $W_0(t)$ and lots of detailed information, and therefore one constructs the representation directly instead of appealing to Theorem XI.82. The construction is accomplished by noticing that for each $\sigma \in \mathbb{R}$ and $\omega \in \mathbb{R}^3$ with $|\omega| = 1$,

$$\varphi_{\sigma, \omega} = e^{-i\sigma\omega \cdot x}\begin{pmatrix} 1 \\ -i\sigma \end{pmatrix}$$

is an (improper) eigenfunction of

$$A_0 = i\begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}$$

with eigenvalue $+\sigma$. Analogously to Section 6, we now define

$$f^*(\sigma, \omega) = (2\pi)^{-3/2}(f, \varphi_{\sigma, \omega})_{\mathscr{H}_0}$$

for $f \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$. We can regard f^* as a function on $\mathbb{R}$ with values in $N = L^2(S^2)$, and it is not hard to show that the map $f \to f^*$ is an isometry of $\mathscr{H}_0$ into $L^2(\mathbb{R}; L^2(S^2))$. In fact the map is unitary and since

$$(A_0 f)^*(\sigma, \omega) = (A_0 f, \varphi_{\sigma, \omega}) = (f, A_0 \varphi_{\sigma, \omega}) = \sigma(f, \varphi_{\sigma, \omega}) = \sigma f^*(\sigma, \omega)$$

A_0 goes over to multiplication by σ. Taking the inverse Fourier transform in the σ variables, one obtains a representation of $\mathscr{H}_0$ as $L^2(\mathbb{R}; L^2(S^2))$ in which $W_0(t)$ is represented as right translation. What is not obvious in this construction is what happens to D_+ and D_-. But it can be shown explicitly that D_+ and D_- go over to $L^2(0, \infty, S^2)$ and $L^2(-\infty, 0; S^2)$, respectively. This shows that the translation representation is both incoming *and* outgoing and, incidentally, that $\mathscr{H}_0 = D_+ \oplus D_-$, a fact that is certainly not obvious in the original representation. This orthogonality gives rise to some of the analyticity properties of the scattering operator which we shall discuss below.

Finally, we remark that the explicit construction of the translation representation can itself be used to provide a proof of Huygens' principle.

Example 2 (acoustic waves in an inhomogeneous medium) Let us consider the first example, (187), of the preceding section from the Lax–Phillips point of view:

$$u_{tt} = c(x)^2 \rho(x) \nabla \cdot \frac{1}{\rho(x)} \nabla u$$

$$u(x, 0) = f(x), \qquad u_t(x, 0) = g(x)$$

We assume all the hypotheses on $c(x)$, $\rho(x)$ that we made in Section 10 and use without comment the spaces and operators H_1, $L^2_{\rho c}(\mathbb{R}^3)$, $\mathscr{H}_1$, B_1, A_1, $W_1(t)$ constructed there. We make one additional assumption on $c(x)$ and $\rho(x)$, namely

$$\rho(x) \equiv 1, \qquad c(x) \equiv 1, \qquad |x| \geq r$$

for some r.

Now, let $r_0 > r$ and let D_+ and D_- be defined as in Example 1. We set

$$D_+^{r_0} \equiv W_0(r_0)D_+, \qquad D_-^{r_0} \equiv W_0(-r_0)D_-$$

Notice that $D_+^{r_0}$, $D_-^{r_0}$ are closed subspaces of $\mathscr{H}_0$. They are also closed subspaces of $\mathscr{H}_1$ since $\varphi \in D_\pm^{r_0}$ implies that φ vanishes inside the ball $B(r_0)$, of radius r_0, so

$$\|\varphi\|_{\mathscr{H}_1} = \|\varphi\|_{\mathscr{H}_0}, \qquad \varphi \in D_\pm^{r_0}$$

since the norms are the same for functions with support outside $B(r)$. We choose J to be the identity operator.

Suppose that $\varphi \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$ and that $\varphi \in D_+^{r_0}$. Since $W_0(t)\colon D_+^{r_0} \to D_+^{r_0}$ for $t \geq 0$, we have

$$(W_0(t)\varphi)' = -iA_0 W_0(t)\varphi = -iA_1 W_0(t)\varphi$$

because A_0 and A_1 coincide on smooth functions with support outside $B(r)$. By the uniqueness of semigroups, $W_0(t)\varphi = W_1(t)\varphi$ for $t \geq 0$ and since such φ are dense in $D_+^{r_0}$, we have

$$W_1(t)\varphi = W_0(t)\varphi, \qquad \varphi \in D_+^{r_0}, \quad t \geq 0 \tag{218}$$

and similarly

$$W_1(t)\varphi = W_0(t)\varphi, \qquad \varphi \in D_-^{r_0}, \quad t \leq 0$$

This shows that W_0 and W_1 satisfy hypotheses (0) and (2) of Theorem XI.86. That condition (3) holds is just what we sketched in Example 1. Further, we know that $D_-^{r_0}$ and $D_+^{r_0}$ are incoming and outgoing subspaces for $W_0(t)$. What we need to show is that they are also incoming and outgoing for $W_1(t)$. By Theorem XI.82, the Lax–Phillips scattering operator $\tilde{S}$ will then exist. And, since hypotheses (0)–(3) of Theorem XI.86 hold, we shall have a new proof that the wave operators exist and are complete, and $(\Omega^-)^{-1}\Omega^+$ will be related to $\tilde{S}$ by (215).

To show that $D_+^{r_0}$ is outgoing for $W_1(t)$, we must verify (i)–(iii). Properties (i) and (ii) follow immediately form (215) and the corresponding statements for the free group proved in Example 1. Property (iii) is much harder and uses a whole array of technical tools. Besides Huygens' principle we shall need a compact embedding theorem of the type discussed in Section XIII.14 and a detailed spectral analysis of A_1. Our plan is to show that (iii) is equivalent to a form of energy decay in the neighborhood of the inhomogeneity and then to prove the energy decay using properties of A_1. Since (iii) implies asymptotic completeness, it is not surprising that it is related to an energy decay condition: We expect asymptotic completeness to hold only if any solution of the interacting equation looks free in the distant future and distant part, that is, if it propagates away from the region of inhomogeneity.

We begin with a lemma which shows that for the free equation, energy propagates at speed one. For any $R > 0$ and $\varphi = \langle u, v\rangle$, define the local energy norms as follows:

$$\|\varphi\|_0^{(R)} \equiv \int_{|x|\le R} |\nabla u|^2 + |v|^2\, dx$$

$$\|\varphi\|_1^{(R)} \equiv \int_{|x|\le R} \rho(x)^{-1}|\nabla u|^2 + (c(x)^2\rho(x))^{-1}|v|^2\, dx$$

Lemma 1

(a) For any $R > 0$,

$$\|W_0(T)\varphi\|_0^{(R)} \le \|\varphi\|_0^{(R+T)} \qquad \text{for all} \quad \varphi \in \mathscr{H}_0$$

(b) For any $R \ge r_0$,

$$\|W_1(T)\varphi\|_1^{(R)} \le \|\varphi\|_1^{(R+T)} \qquad \text{for all} \quad \varphi \in \mathscr{H}_1$$

Proof The idea is to integrate an "energy flux" over the surface of the region $\Omega(R, T)$ given by $|x| \le R + T - t$, $0 \le t \le T$, shown in Figure XI.14. Because of conservation of energy, no net flux can be produced inside $\Omega(R, T)$, and because of the finite propagation speed, flux can flow only out of the sides; so the flux in at the bottom $\|\cdot\|_i^{(R+T)}$ must be greater than the flux out at the top $\|W_i(T)\cdot\|_i^{(R)}$.

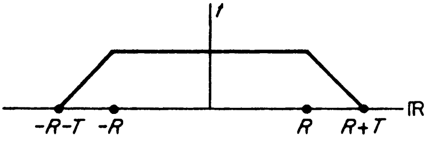


FIGURE XI.14 $\Omega(R, T)$.

Explicitly, define

$$j_0(x, t) = \tfrac{1}{2}[(c^2(x)\rho(x))^{-1}|u_t(x, t)|^2 + \rho(x)^{-1}|\nabla u(x, t)|^2]$$
$$j_i(x, t) = -\rho(x)^{-1}\operatorname{Re}\{\overline{u_t}(x, t)\,\partial_i u(x, t)\}$$

and set $j = \langle j_0, \mathbf{j}\rangle$. We will see in the appendix to Section 13 that these are four of the components of the energy-momentum tensor. Suppose first that $\varphi = \langle f, g\rangle$ with $f, g \in C_0^\infty$. Let $u(x, t) = (W_1(t)\varphi)_1$. Standard arguments of the type used in Section X.13 show that u is C^∞ in x and t. A direct calculation using $u_{tt} = c^2\rho\nabla \cdot \rho^{-1}\nabla u$ shows that

$$\nabla_{\mathbf{R}^4} \cdot j = \frac{\partial j_0}{\partial t} + \sum_{i=1}^{3} \frac{\partial j_i}{\partial x_i} = 0$$

So, by Gauss's theorem,

$$\int_{\partial\Omega(R,\,T)} j \cdot \sigma \, dS = 0$$

where $\sigma = \langle \sigma_0, \boldsymbol{\sigma} \rangle$ is the outward pointing normal and dS is the surface measure. By the inequality $2ab \le a^2 + b^2$, $|\mathbf{j}(x, t)| \le j_0(x, t)$ at points where $c = 1$, such as the sides of Ω. Moreover, $|\boldsymbol{\sigma}(x, t)| = \sigma_0(x, t)$ on the sides of Ω. It follows that $j \cdot \sigma \ge 0$ on the sides of Ω so

$$\int_{|x| \le R} j_0(x, T)\, dx \le \int_{|x| \le R + T} j_0(x, 0)\, dx$$

which proves (b) for smooth φ. A limiting argument proves (b) for all $\varphi \in \mathscr{H}_1$. A similar argument proves (a). ▮

With this lemma, we can now show that (iii) is equivalent to a weak form of local energy decay.

Lemma 2 Under the hypotheses in Example 2, (iii) holds if and only if

$$\underline{\lim}_{t \to +\infty} \| W_1(t)\varphi \|_1^{(R)} = 0 \tag{219}$$

for all $\varphi \in \mathscr{H}_1$ and all $R < \infty$.

Proof First, suppose that (iii) holds. Then, given any $\varphi \in \mathscr{H}_1$ and $\varepsilon > 0$, there is a t_0 and a $\psi \in D_+^{r_0}$ so that $\| W_1(t_0)\psi - \varphi \|_1 \le \varepsilon$. Now, since $\psi \in D_+^{r_0}$, $W_1(t + t_0)\psi$ vanishes in $B(R)$ if $t > R - t_0$. Thus since

$$\| W_1(t)\varphi - W_1(t + t_0)\psi \|_1 = \| \varphi - W_1(t_0)\psi \|_1 \le \varepsilon$$

for all t, we have

$$\| W_1(t)\varphi \|_1^{(R)} \le \varepsilon \qquad \text{for} \quad t \ge R - t_0$$

Therefore $\lim_{t\to\infty} \| W_1(t)\varphi \|_1^{(R)} = 0$, which is a priori stronger than (219).

To prove the converse, suppose that (219) holds and that ψ is perpendicular to $\overline{\bigcup W_1(t) D_+^{r_0}}$, which is the same as saying that $W_1(t)\psi \perp D_+^{r_0}$ for all t. From the fact that the free translation representation of $D_+^{r_0}$ is all of

$L^2(r_0, \infty; N)$, we conclude that $W_0(-2r_0)W_1(t)\psi \in D_-^{r_0}$ for all t. Since $W_1(-s)$ and $W_0(-s)$ agree on $D_-^{r_0}$ for $s \geq 0$, we have

$$W_0(-(s+2r_0))W_1(t)\psi = W_1(-s)W_0(-2r_0)W_1(t)\psi \tag{220}$$

and also that $W_0(-s)W_1(t)\psi$ is zero for $|x| < s - r_0$.

Now, given $\varepsilon > 0$, by (219) we can find a $t > (k+1)r_0$ such that

$$\|W_1(t)\psi\|_1^{(5r_0)} < \varepsilon$$

so by Lemma 1,

$$\|W_0(-2r_0)W_1(t)\psi\|_1^{(3r_0)} \leq d\|W_0(-2r_0)W_1(t)\psi\|_0^{(3r_0)} \leq d_0\varepsilon$$

$$\|W_1(t-2r_0)\psi\|_1^{(3r_0)} \leq \varepsilon$$

where d_0 is a universal constant relating the two equivalent norms $\|\cdot\|_1$ and $\|\cdot\|_0$. Notice that $W_0(-s)W_1(t)\psi = W_1(-s)W_1(t)\psi$ at $s = 0$, and thus these two solutions will be equal for $|x| > |s| + r_0$ since the solution at such points is not affected by the inhomogeneity inside $B(r_0)$. In particular,

$$(W_0(-2r_0)W_1(t)\psi)(x) = (W_1(-2r_0)W_1(t)\psi)(x)$$

for $|x| > 3r_0$. This fact and the estimates above imply that

$$\|W_0(-2r_0)W_1(t)\psi - W_1(t-2r_0)\psi\|_1 \leq (1+d_0)\varepsilon$$

Now set $s = t - 2r_0$. Since $W_1(2r_0 - t)$ is unitary, we have (using (220))

$$\|W_0(-t)W_1(t)\psi - \psi\|_1 \leq (1+d_0)\varepsilon$$

But recall that $W_0(-t)W_1(t)\psi$ is zero for $|x| < t - r_0$. Choosing $t > (k+1)r_0$, we have that

$$\|\psi\|_1^{(kr_0)} \leq (1+d_0)\varepsilon$$

Since ε and k are arbitrary, we conclude that $\psi = 0$. Thus (iii) holds. ▌

To prove (219), we need a local compactness result.

Lemma 3 Fix c_1. The set $\mathscr{K}$ of $\varphi \in D(A_1)$ such that $\|A_1\varphi\|_1 + \|\varphi\|_1 \leq c_1$ is compact in the $\|\cdot\|_1^{(R)}$-norm for each R; that is, given any sequence in $\mathscr{K}$, there is a subsequence converging in the $\|\cdot\|_1^{(R)}$-norm.

Proof Let $\varphi = \langle u, v\rangle$. The condition of the hypothesis says that

$$\|B_1^2 u\|_{\rho c}^2 + \|B_1 u\|_{\rho c}^2 + \|B_1 v\|_{\rho c}^2 + \|v\|_{\rho c}^2 \leq c_1$$

for some c_1. Using the conditions (190) on c and ρ, one easily obtains from this that

$$\|\Delta u\|_2^2 + \|\nabla u\|_2^2 + \|\nabla v\|_2^2 + \|v\|_2^2 \leq c_2$$

for all φ in the original set $\mathscr{K}$. By Corollary 1 to Theorem XIII.74, the set of $v \in L^2$ satisfying $\|\nabla v\|_2^2 + \|v\|_2^2 \leq c_2$ is compact in the local norm $\|v\|_2^{(R)}$; and similarly, the set satisfying $\|\Delta u\|_2^2 + \|\nabla u\|_2^2 \leq c_2$ is compact in the local norm $\|\nabla u\|_2^{(R)}$. Thus $\mathscr{K}$ is compact in the local norm $\|\cdot\|_0^{(R)}$, and therefore also in $\|\cdot\|_1^{(R)}$ since the norms are equivalent. ▮

Finally, we need spectral information on A_1.

Lemma 4 A_1 has purely absolutely continuous spectrum.

Proof This will clearly be true if $B_1^2 = -c(x)^2\rho(x)\nabla \cdot \rho(x)^{-1}\nabla$ has purely absolutely continuous spectrum on $L^2_{\rho c}(\mathbb{R}^3)$. B_1^2 is unitarily equivalent to the operator

$$\tilde{B}_1^2 = -(c(x)^2\rho(x))^{1/2} \circ \nabla \cdot \rho(x)^{-1}\nabla \circ (c(x)^2\rho(x))^{1/2}$$

on $L^2(\mathbb{R}^3)$. In Theorem XIII.62 we shall show that such an operator has no eigenvalues. In Theorem XI.45 we showed that matrix elements of the resolvent are bounded for a dense set of vectors as one approaches the real axis. This fact implies that there is no singular continuous spectrum (Theorem XIII.19). ▮

We are now ready to complete the argument and prove (iii). Let φ be in $D(A_1)$ and consider the set $\mathscr{K}_\varphi = \{U_1(t)\varphi \mid t \in \mathbb{R}\}$. Since

$$\|A_1 U_1(t)\varphi\|_1 + \|U_1(t)\varphi\|_1 = \|A_1\varphi\|_1 + \|\varphi\|_1$$

$\mathscr{K}_\varphi$ is compact in $\|\cdot\|_1^{(R)}$ by Lemma 3. Moreover, A_1 has purely absolutely continuous spectrum, so $(U_1(t)\varphi, \psi)_1 \to 0$ as $t \to +\infty$ for all φ, ψ by the Riemann–Lebesgue lemma. It follows that any $\|\cdot\|_1^{(R)}$ limit point must be zero, so, by the compactness,

$$\lim_{t \to +\infty} \|U_1(t)\varphi\|_1^{(R)} = 0$$

Since $D(A_1)$ is dense in $\mathscr{H}_1$ and $U_1(t)$ is unitary, this holds for all $\varphi \in \mathscr{H}_1$ and all $R > 0$ which, by Lemma 2, proves (iii). We summarize:

Theorem XI.88 Let $c(x)$ and $\rho(x)$ be smooth functions that equal constants outside of a compact set and satisfy (190). Then $D_+^{r_0}$ and $D_-^{r_0}$ are outgoing and incoming subspaces for $W_1(t) = e^{-iA_1t}$ on $\mathscr{H}_1$, so by Theorem XI.82, the Lax–Phillips scattering operator exists. Further, for any identification operator $J: \mathscr{H}_0 \to \mathscr{H}_1$ which is the identity on $D_\pm^{r_0}$, the wave operators $\Omega^\pm(A_0, A_1, J)$ exist, are complete, and are related to the Lax–Phillips scattering operator by the formula (215).

It is worthwhile to point out here an important difference between the Lax–Phillips approach and that of Section 10. In order to construct the Lax–Phillips scattering operator, we needed the fact that A_1 has purely absolutely continuous spectrum; actually, with a longer argument (the RAGE theorem), purely continuous spectrum is enough. Except for constant coefficient operators where one can use the Fourier transform, the elimination of point spectrum is a hard problem (see Theorem XIII.62). Thus the Lax–Phillips approach requires quite delicate information about the generator of the interacting dynamics. This information is not required for the approach of Section 10, which uses the Kato–Birman theory. Of course, the conclusion we got there was weaker in that we knew only that $\operatorname{Ran}\Omega^+ = \mathscr{H}_{\mathrm{ac}}(A_1) = \operatorname{Ran}\Omega^-$, and not $\mathscr{H}_{\mathrm{ac}}(A_1) = \mathscr{H}_1$. But $\operatorname{Ran}\Omega^+ = \operatorname{Ran}\Omega^-$ is all that one needs to construct the scattering operator itself.

We now return to the abstract theory and investigate properties of the scattering operators $\tilde{S}$ and $\hat{S} = \mathscr{F}\tilde{S}\mathscr{F}^{-1}$ on $L^2(\mathbb{R}; N)$.

Proposition Let D_+ and D_- be outgoing and incoming subspaces for a unitary group $U(t)$ on $\mathscr{H}$. Then:

(a) The scattering operator $\tilde{S}$ on $L^2(\mathbb{R}; N)$ commutes with translation.
(b) If D_+ and D_- are orthogonal to each other, then

$$\tilde{S}\colon L^2(-\infty, 0; N) \to L^2(-\infty, 0; N)$$

Proof Let $\mathscr{R}_\pm$ be the maps onto the outgoing and incoming translation representations of $\mathscr{H}$, $U(t)$, $D^\pm$. Then

$$\tilde{S}T_0(s) = \mathscr{R}_+\mathscr{R}_-^{-1}T_0(s) = \mathscr{R}_+U(s)\mathscr{R}_-^{-1} = T_0(s)\mathscr{R}_+\mathscr{R}_-^{-1} = T_0(s)\tilde{S}$$

where $T_0(s)$ is translation by s units. This proves (a). (b) is also easy. For if $f \in L^2(-\infty, 0; N)$, then $\mathscr{R}_-^{-1}f \in D_-$ and since D_- is orthogonal to D_+ we know that $\tilde{S}f = \mathscr{R}_+\mathscr{R}_-^{-1}f$ is orthogonal to $\mathscr{R}_+D_+$. But, $\mathscr{R}_+D_+ \equiv L^2(0, \infty; N)$, so $\tilde{S}f \in L^2(-\infty, 0; N)$. ∎

As we have already noted, if (0)–(3) hold, then $D_+^{r_0}$ and $D_-^{r_0}$ are *orthogonal* outgoing and incoming subspaces for $U(t)$. Some analyticity of $\hat{S}$ follows from the following general theorem.

Theorem XI.89 Let N be a separable Hilbert space and T a bounded operator on $L^2(\mathbb{R}; N)$ such that T commutes with translation and takes $L^2(-\infty, 0; N)$ into itself. Then, $\hat{T} = \mathscr{F}T\mathscr{F}^{-1}$ operates on $L^2(\mathbb{R}; N)$ by multiplication by an $\mathscr{L}(N)$-valued function $t(\sigma)$:

$$(\hat{T}f)(\sigma) = t(\sigma)f(\sigma) \tag{221}$$

Further, there is a norm analytic $\mathscr{L}(N)$-valued function $t(\sigma + iy)$ in the open upper half-plane so that:

(a) $\|t(\sigma + iy)\|_{\mathscr{L}(N)} \le \|T\|, \sigma \in \mathbb{R}, y > 0;$
(b) $t(\sigma + iy)$ converges weakly to $t(\sigma)$ for almost all $\sigma \in \mathbb{R}$ as $y \downarrow 0$.

Proof We consider first the case where $N = \mathbb{C}$. Suppose that T is an operator on $L^2(\mathbb{R}; \mathbb{C})$ that commutes with translations. We first claim that (221) holds. Given (221), it is clear that $t \in L^\infty$ and $\|t\|_\infty = \|\hat{T}\| = \|T\|$.

There are two different ways of proving (221). First note that T is a linear map of $\mathscr{S}(\mathbb{R})$ into $L^2(\mathbb{R})$. Since T commutes with translations, it is easy to check that T is actually a continuous map of $\mathscr{S}(\mathbb{R})$ into $C^\infty(\mathbb{R})$. Thus, by Problem 9 of Chapter IX, there is a distribution $\tau \in \mathscr{S}'$ such that

$$T(f) = \tau * f$$

for $f \in \mathscr{S}(\mathbb{R})$. Thus there is a distribution $t \in \mathscr{S}'$ such that (221) holds for $f \in \mathscr{S}$. Since

$$\left| \int \overline{g(\sigma)} t(\sigma) f(\sigma)\, d\sigma \right| = |(g, \hat{T}f)| \le \|\hat{T}\|\, \|g\|_2 \|f\|_2$$

we conclude that t is a bounded function and (221) holds for all $f \in L^2(\mathbb{R})$. The second proof argues that since T commutes with translation, $\hat{T}$ commutes with multiplication by $e^{i\sigma a}$ for all a. By a limiting argument, $\hat{T}$ commutes with multiplication by any bounded measurable function. (221) then follows immediately from Theorem XIII.84.

The first step in proving the analyticity is to show that τ has support on $(-\infty, 0]$. Let j be a positive function in $C_0^\infty(-\infty, 0)$ with $\int j(x)\, dx = 1$ and define $j_\delta(x) = \delta^{-1} j(x/\delta)$, $\tau_\delta = \tau * j_\delta$. Then

$$f \mapsto \tau_\delta * f = T(j_\delta * f)$$

takes $L^2(-\infty, 0)$ to itself. If we can show that each τ_δ has support in $(-\infty, 0]$, then so does τ since $\tau_\delta \to \tau$. Thus, it suffices to prove the support property in the case where τ is a C^∞ function. Suppose that $\tau(a) \ne 0$ for some $a > 0$. Then we can find δ and θ so that $\mathrm{Re}(e^{i\theta}\tau(x)) > 0$ for all $x \in (a - \delta, a + \delta)$. Letting f be the characteristic function of $(-\delta, 0)$, we see that $\mathrm{Re}\{e^{i\theta}(\tau * f)(x)\} > 0$ for $x \in (a, a + \delta)$, which violates the hypothesis that T leaves $L^2(-\infty, 0)$ invariant. Thus τ has support on $(-\infty, 0]$.

Since τ has support on the half-line, Theorem IX.16 implies that t is the boundary value in the sense of distributions of an analytic function $t(\sigma + iy)$ in the upper half-plane satisfying

$$|t(\sigma + iy)| \le C(1 + \sigma^2 + y^2)^{N_1}(1 + y^{-N_2})$$

for some C, N_1, and N_2. We want to show that t is bounded in the upper half-plane with $\|t\|_\infty \le \|T\|$. Let $\tau_\varepsilon(x) = (2\pi)^{1/2}e^{-\varepsilon x^2}\tau(x)$ and define

$$t_\varepsilon(\sigma + iy) \equiv (2\pi)^{-1/2} \int \tau_\varepsilon(x)e^{-i(\sigma+iy)x}\, dx$$

$$= \int t(\sigma + iy - \mu)\frac{e^{-\mu^2/4\varepsilon}}{\sqrt{4\pi\varepsilon}}\, d\mu$$

Then, for fixed $y > 0$, $t_\varepsilon(\cdot + iy) \to t(\cdot + iy)$ pointwise, so it suffices to show that $\|t_\varepsilon(\cdot + iy)\|_\infty \le \|T\|$ for each ε and y. Now, since τ is tempered, it is the Nth derivative of a polynomially bounded continuous function h. It follows that t_ε is entire and

$$|t_\varepsilon(\sigma + iy)| = \int |[D^N h](e^{-\varepsilon x^2}\, e^{-i(\sigma+iy)x})|\, dx$$

$$\le C(1 + |\sigma + iy|)^N$$

Let $\delta > 0$ be a given small number, and define

$$t_{\varepsilon,\delta}(\sigma + iy) = (1 - i\delta(\sigma + iy))^{-N}t_\varepsilon(\sigma + iy)$$

If $Y \ge 2\delta^{-1} + 1$, then

$$\frac{1 + |\sigma + iY|}{|1 - i\delta(\sigma + iY)|} \le \frac{2}{\delta}$$

for all σ, so

$$\|t_{\varepsilon,\delta}(\cdot + iY)\|_\infty \le C\left(\frac{2}{\delta}\right)^N$$

and

$$\|t_{\varepsilon,\delta}(\cdot + i0)\|_\infty \le \|t_\varepsilon(\cdot + i0)\|_\infty \le \|T\|$$

Since $t_{\varepsilon,\delta}$ is bounded, Hadamard's three lines theorem implies that

$$\|t_{\varepsilon,\delta}(\cdot + iy)\|_\infty \le \|T\|^{1-y/Y}\left[C\left(\frac{2}{\delta}\right)^N\right]^{y/Y}$$

for each y satisfying $0 < y < Y$. Holding y fixed and taking Y to infinity, we see that

$$\|t_{\varepsilon,\delta}(\cdot + iy)\|_\infty \le \|T\|$$

Finally, letting $\delta \to 0$ and then $\varepsilon \to 0$, we conclude that $\|t(\cdot + iy)\|_\infty \le \|T\|$ for each $y > 0$.

Continuity at the real axis follows from a general complex variables result which we state after the theorem.

Now let N be an arbitrary Hilbert space. For $\varphi, \eta \in N$,

$$T_{\varphi,\eta}: f \to (\varphi, T(f\eta))_N$$

maps $L^2(\mathbb{R})$ into itself and $L^2(-\infty, 0)$ into itself. So, by the scalar case,

$$\widehat{T_{\varphi,\eta}(\check{f})} = t_{\varphi,\eta}(\sigma) f(\sigma)$$

where $t_{\varphi,\eta}(\sigma + iy)$ is analytic in the upper half-plane, has $t_{\varphi,\eta}(\sigma)$ as boundary value, and satisfies

$$|t_{\varphi,\eta}(\sigma + iy)| \leq \|T_{\varphi,\eta}\| \leq \|T\| \; \|\varphi\|_N \; \|\eta\|_N$$

in the closed upper half-plane. Since $\langle\varphi, \eta\rangle \to T_{\varphi,\eta}$ is sesquilinear, so is $\langle\varphi, \eta\rangle \to t_{\varphi,\eta}(\sigma + iy)$ for each σ and $y \geq 0$. Thus, by the Riesz lemma, for each $\sigma + iy$, there is a bounded operator $t(\sigma + iy)$ on N so that

$$t_{\varphi,\eta}(\sigma + iy) = (\varphi, t(\sigma + iy)\eta)_N$$

$t(\sigma + iy)$ is clearly weakly analytic and multiplication by $t(\sigma)$ on $L^2(\mathbb{R}; N)$ is $\mathscr{F} T \mathscr{F}^{-1}$. Norm analyticity follows from the fact that $\|t(\sigma + iy)\|$ is uniformly bounded and the methods of Theorem VI.4 (Problem 123). Since $t_{\varphi,\eta}(\sigma + iy)$ has $t_{\varphi,\eta}(\sigma)$ as its pointwise limit as $y \downarrow 0$ for almost all σ, $t(\sigma + iy)$ has $t(\sigma)$ as its limit in the weak operator topology on N for almost all σ. ▌

In the above proof, continuity up to the axis follows from the following result (see the reference in the Notes):

Lemma (Fatou's theorem) If $F(z)$ is analytic in the upper half-plane and

$$\sup_{y>0} \int |F(x + iy)|^p \, dx < \infty$$

for some $p > 1$ (where $p = \infty$ is allowed), then for almost all $x \in \mathbb{R}$,

$$\lim_{y \downarrow 0} F(x + iy) \equiv f(x)$$

exists, $f \in L^p$, and $F(\cdot + iy) \to f(\cdot)$ in the sense of distributions.

Applying Theorem XI.89 to the case we are interested in, we have:

Corollary Suppose that there exist orthogonal incoming and outgoing subspaces for a unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Then, there is an $\mathscr{L}(N)$-valued function $s(\sigma + iy)$ on the closed upper half-plane satisfying:

(1) $s(\sigma + i0)$ is unitary almost everywhere.

(2) $s(\sigma + iy)$ is norm analytic in the open upper half-plane with

$$\|s(\sigma + iy)\|_{\mathscr{L}(N)} \leq 1$$

(3) $s(\sigma + iy)$ converges strongly to $s(\sigma)$ almost everywhere as $y \downarrow 0$ and, for all $f \in L^2(\mathbb{R}; N)$,

$$(\hat{S}f)(\sigma) = s(\sigma)f(\sigma)$$

and $\hat{S}$ takes $\mathscr{H}^2_+(\mathbb{R}; N)$ into itself.

Proof All the statements of the theorem except *strong* continuity up to the real axis follow immediately from Theorem XI.89 and the previous proposition. Strong continuity follows from weak continuity since

$$\begin{aligned}\|s(\sigma + iy)\varphi - s(\sigma)\varphi\|_N^2 &= \|s(\sigma + iy)\varphi\|_N^2 - (s(\sigma + iy)\varphi, s(\sigma)\varphi)_N \\ &\quad - (s(\sigma)\varphi, s(\sigma + iy)\varphi)_N + \|s(\sigma)\varphi\|_N^2 \\ &\to 0\end{aligned}$$

because $\|s(\sigma + iy)\| \leq 1 = \|s(\sigma)\|$. ▮

As in the quantum-mechanical case discussed in Section 7, the analytic continuation properties of the scattering operator are important. Thus one wants general methods for investigating the continuation properties of $s(z)$. Since $s(z)$ is unitary on the real axis, the natural way to try to continue it to the lower half-plane is by the formula

$$s(z) = [s(\bar{z})^*]^{-1}, \qquad \operatorname{Im} z < 0$$

But for this formula to work we need to know that zero is in the resolvent set of $s(\bar{z})$, that is, that $s(\bar{z})$ is *regular*. In order to do this, Lax and Phillips introduced the following semigroup:

Let $\mathscr{K} = (D_+ \oplus D_-)^\perp$ and let $P_{\mathscr{K}}$ be the orthogonal projection onto $\mathscr{K}$. Define

$$Z(t) = P_{\mathscr{K}} U(t) P_{\mathscr{K}}, \qquad t \geq 0 \tag{222}$$

$Z(t)$ is clearly the restriction of the dynamics to the states that are neither incoming in the past nor outgoing in the future, so it is not surprising that it will contain information about resonances. $Z(t)$ is obviously a strongly continuous family of contraction operators. Moreover, if $\varphi, \psi \in \mathscr{K}$ and $t, s \geq 0$, then $U(t)\varphi \in D_+^\perp$ and $U(-s)\psi \in D_-^\perp$ (since $U(t)$ leaves $D_\pm$ invariant for $\pm t \geq 0$). So

$$(U(-s)\varphi, P_{\mathscr{K}} U(t)\psi) = (U(-s)\varphi, U(t)\psi), \qquad t, s \geq 0$$

since $P_{\mathscr{K}} = P_- P_+$ where P_+ (respectively, P_-) is the projection onto the orthogonal *complement* of D_+ (respectively, D_-). Equivalently, $P_{\mathscr{K}} U(s) P_{\mathscr{K}} U(t) P_{\mathscr{K}} = P_{\mathscr{K}} U(s+t) P_{\mathscr{K}}$ or $Z(t)Z(s) = Z(t+s)$. Thus, $Z(t)$ is a strongly continuous group of contractions on $\mathscr{K}$, and therefore there is an m-accretive operator B on $\mathscr{K}$ with $\sigma(B) \subset \{z \mid \operatorname{Re} z > 0\}$ such that

$$Z(t) = e^{-Bt}$$

Since $U(t)$ has absolutely continuous spectrum,

$$(Z(t)\varphi, \psi) \to 0 \qquad \text{as} \quad t \to \infty \tag{223}$$

Moreover

$$Z(t) = P_+ U(t) P_-, \qquad t \geq 0 \tag{224}$$

For since $U(t)$ leaves D_+ invariant, $P_+ U(t) P_+ = P_+ U(t)$; and since $U(-t)$ leaves D_- invariant, $P_- U(t) P_- = U(t) P_-$; so

$$P_{\mathscr{K}} U(t) P_{\mathscr{K}} = P_- P_+ U(t) P_+ P_- = P_+ P_- U(t) P_- = P_+ U(t) P_-$$

The semigroup $Z(t)$ is important because the resolvent set of B is simply related to the invertibility of $s(z)$.

Theorem XI.90 Let D_+ and D_- be orthogonal outgoing and incoming subspaces for a unitary group $U(t)$ on a Hilbert space $\mathscr{H}$. Let $Z(t) = e^{-Bt}$ be defined by (222). Then, if $\operatorname{Re} z > 0$, $z \in \rho(B)$ if and only if $s(i\bar{z})$ is regular.

We shall sketch the proof that $s(i\bar{z}_0)^*$ has a zero eigenvalue if and only if B has z_0 as an eigenvalue. By definition,

$$\begin{aligned} \mathscr{K} &= \{\chi \mid \mathscr{R}_+ \chi \in L^2(-\infty, 0; N); \mathscr{R}_- \chi \in L^2(0, \infty; N)\} \\ &= \{\chi \mid \mathscr{R}_+ \chi \in L^2(-\infty, 0; N); \tilde{S}(\mathscr{R}_- \chi) = \mathscr{R}_+ \chi \in \tilde{S} L^2(0, \infty; N)\} \end{aligned}$$

Thus

$$\mathscr{R}_+[\mathscr{K}] \equiv \mathscr{K}_+ = \{f \mid f \in L^2(-\infty; 0; N), \tilde{S}^* f \in L^2(0, \infty; N)\}$$

Next, let $Z_+(t) = \mathscr{R}_+ Z(t) \mathscr{R}_+^{-1}$ and note that for $f \in \mathscr{K}_+$,

$$\begin{aligned} Z_+(t) f &= (\mathscr{R}_+ P_+ \mathscr{R}_+^{-1})(T_0(t) f) \\ &= \chi_{(-\infty, 0)} T_0(t) f \end{aligned}$$

That is, if $f \in \mathscr{K}_+$,

$$(Z_+(t) f)(s) = \begin{cases} f(s-t), & \text{if} \quad s \leq 0 \\ 0, & \text{if} \quad s > 0 \end{cases}$$

Now, $Bx = z_0 x$ if and only if $Z(t)x = e^{-z_0 t}x$. Moreover, $f(s-t) = e^{-z_0 t}f(s)$ $(s \le 0)$ if and only if $f(s) = e^{z_0 s}\chi_{(-\infty,0)}(s)n$ for some $n \in N$. Thus z_0 is an eigenvalue of B if and only if $e^{z_0 s}\chi_{(-\infty,0)}(s)n \equiv f_0$ is in $\mathscr{K}_+$ for some $n \in N$. Since f_0 is clearly in $L^2(-\infty, 0; N)$, $f_0 \in \mathscr{K}_+$ if and only if $\tilde{S}^* f_0$ is in $L^2(0, \infty; N)$. This is true if and only if $s(\bar{z})^* \hat{f}_0(z)$ is analytic in the lower half-plane. But $\hat{f}_0(z) = (2\pi)^{-1/2}(z_0 - iz)^{-1}n$ has a pole at $z = -iz_0$, so $s(\bar{z})^* \hat{f}_0(z)$ will be analytic in the lower half-plane if and only if $s(i\bar{z}_0)^* n = 0$. This completes the proof of one part of Theorem XI.90 and illustrates the reasons the theorem is valid.

Example 3 We consider a trivial example to illustrate Theorem XI.90. Let $U(t)$ be translation on $L^2(-\infty, \infty)$. Fix $r_0 > 0$, and let $D_+ = L^2(r_0, \infty)$, $D_- = L^2(-\infty, -r_0)$. Then D_+ is outgoing, D_- is incoming and, by a simple calculation, $\tilde{S} = U(-2r_0)$ and $s(k) = e^{2ikr_0}$. s is clearly entire. Notice that D_+ and D_- are orthogonal and that $\mathscr{K} = L^2(-r_0, r_0)$. It follows that $Z(t) = 0$ if $t > 2r_0$. In particular,

$$(B + \lambda)^{-1} = \int_0^\infty Z(t) e^{-\lambda t}\, dt$$

extends from $\operatorname{Re} \lambda > 0$ to an entire function. Thus $\sigma(B) = \varnothing$ which is as required by Theorem XI.90.

Theorem XI.90 reduces the analyticity question to studying B.

Theorem XI.91 Suppose that for some positive T and k, $Z(T)(k + B)^{-1}$ is compact. Then B has pure point spectrum and $s(z)$ is holomorphic on the real axis and has a meromorphic extension to the lower half-plane, having a pole at each z for which $iz \in \sigma(B)$.

The idea of the proof of this theorem is to use a spectral mapping theorem to show that B has pure point spectrum. By Theorem XI.90, $s(z)$ is invertible in the upper half-plane except when $i\bar{z}$ is an eigenvalue for B. Thus

$$s(z) = [s(\bar{z})^*]^{-1}$$

is analytic in the lower half-plane except for z for which iz is an eigenvalue of B. By the above expression, $s(z)$ can only have poles since $s(\bar{z})^*$ can only have zeros of finite order. Finally, by (223), B cannot have any eigenvalues with $\operatorname{Re} \mu = 0$. From this it follows that $(s(\bar{z})^*)^{-1}$ is analytic in an open set just below the real axis. Since $s(z)$ and $(s(\bar{z})^*)^{-1}$ have the same bounded boundary values as one approaches the real axis from above and below, they are analytic continuations of each other by the Schwartz reflection principle. Thus $s(z)$ is analytic in a neighborhood of the real axis and meromorphic in the lower half-plane.

For complete proofs of Theorems XI.90 and XI.91, see the reference in the Notes.

Example 4 The purpose of this example is to show how the hypotheses of Theorem XI.91 may be verified in practice. We shall deal with the case of scattering off an obstacle Ω with smooth boundary and Dirichlet boundary conditions discussed in Example 3 of Section 10. We use the notation introduced there. The operator A_1 for this problem is the Laplacian $H_{\Gamma;\,D}$ of Section XIII.15. We prove the absence of singular continuous spectrum in an appendix to this section. With this result, the analysis of Example 2 extends to this case. In their treatment, Lax and Phillips do not require a priori the absence of singular continuous spectrum. Instead, they prove (3) by a more difficult argument and then obtain the absence of singular continuous spectrum as a result of Theorem XI.82. The technique that we describe here can also be used to prove the hypotheses of Theorem XI.91 in the case of scattering in an inhomogeneous medium (Example 2), but the proofs are more difficult because the natural identification operator is not isometric (Problem 124).

D_+ and D_- are, as in Example 1, the incoming and outgoing subspaces for the free propagation $W_0(t)$. Let r_0 be chosen so that the ball $B(r_0)$ contains Ω in its interior and define

$$D_+^{r_0} = W_0(r_0)D_+, \qquad D_-^{r_0} = W_0(-r_0)D_-$$

Since the functions in $D_+^{r_0}$ and $D_-^{r_0}$ vanish in $B(r_0)$, $D_+^{r_0}$ and $D_-^{r_0}$ are subspaces of $\mathscr{H}_0$ that are isometrically imbedded in $\mathscr{H}_1$. One can show that $D_+^{r_0}$ and $D_-^{r_0}$ are outgoing and incoming subspaces for $W_1(t)$ on $\mathscr{H}_1$ and that the hypotheses of Theorem XI.86 hold. In particular, $D_\pm^{r_0}$ are orthogonal. Let $P_\pm^{r_0}$ be the projections onto $(D_\pm^{r_0})^\perp$ in $\mathscr{H}_1$ and define $Z(t) = P_+^{r_0}\, W_1(t)P_-^{r_0}$. Suppose that $\varphi \in \mathscr{H}_1$ and $\mu > 0$. Then, by (X.98),

$$
\begin{aligned}
Z(2r_0)(\mu + B)^{-1}\varphi &= \int_0^\infty e^{-\mu t} Z(t + 2r_0)\varphi\, dt \\
&= P_+^{r_0}\, W_1(2r_0) \int_0^\infty e^{-\mu t} W_1(t) P_-^{r_0}\varphi\, dt \\
&= iP_+^{r_0}\, W_1(2r_0)(i\mu - A_1)^{-1} P_-^{r_0}\varphi \\
&= iP_+^{r_0}\, W_1(2r_0)P_-^{r_0}(i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (225) \\
&= iP_+^{r_0}[W_1(2r_0) - W_0(2r_0)]P_-^{r_0} \\
&\quad \times (i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (226) \\
&= iP_+^{r_0}[W_1(2r_0) - W_0(2r_0)] \\
&\quad \times (i\mu - A_1)^{-1} P_-^{r_0}\varphi \qquad (227)
\end{aligned}
$$

Steps (225) and (227) follow from the fact that for $t \geq 0$, $P_-^{r_0} W_1(t) P_-^{r_0} = W_1(t) P_-^{r_0}$, from which it follows that

$$P_-^{r_0}(i\mu - A_1)^{-1} P_-^{r_0} = (i\mu - A_1)^{-1} P_-^{r_0}$$

Step (226) holds because $P_+^{r_0} W_0(2r_0) P_-^{r_0} = 0$. To see this notice that for any $f \in \mathscr{H}_1$, $P_-^{r_0} f$ is orthogonal to $D_-^{r_0}$ in $\mathscr{H}_0$ because $\mathscr{H}_1$ is isometrically imbedded in $\mathscr{H}_0$. Thus the free translation representative of $P_-^{r_0} f$ has support on $(-r_0, \infty)$. Therefore, the representative of $W_0(2r_0) P_-^{r_0} f$ has support on (r_0, ∞), which implies that $W_0(2r_0) P_-^{r_0} f$ is in $D_+^{r_0}$.

Now, for any $g \in \mathscr{H}_1$,

$$W_0(2r_0)g - W_1(2r_0)g = 0 \qquad \text{for} \quad |x| \geq 3r_0$$

since the propagation speed is one. Thus, using the fact that $\|\psi\|_0 = \|\psi\|_1$, we can estimate

$$\begin{aligned}
\|Z(2r_0)(\mu + B)^{-1}\varphi\|_1 &\leq \|[W_1(2r_0) - W_0(2r_0)](i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_0 \\
&= \|[W_1(2r_0) - W_0(2r_0)](i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_0^{(3r_0)} \\
&\leq \|W_1(2r_0)(i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_1^{(3r_0)} \\
&\quad + \|W_0(2r_0)(i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_0^{(3r_0)} \\
&\leq \|(i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_1^{(5r_0)} + \|(i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_0^{(5r_0)} \\
&= 2\|(i\mu - A_1)^{-1} P_-^{r_0} \varphi\|_1^{(5r_0)}
\end{aligned}$$

where $\|\cdot\|^{(R)}$ denotes the part of the norm inside the ball of radius R. In the next to last step we used part (a) of Lemma 1 in Example 2 and an analogous result for $W_1(t)$ (the proof is similar). The set of $\psi = (i\mu - A_1)^{-1}\varphi$ where $\|\varphi\| \leq 1$, satisfies

$$\|A_1\psi\|_1 + \|\psi\|_1 \leq \|A_1(i\mu - A_1)^{-1}\|_{\mathscr{L}(\mathscr{H}_1)} + \|(i\mu - A_1)^{-1}\|_{\mathscr{L}(\mathscr{H}_1)}$$

Therefore, using Corollary 2 to Theorem XIII.74, we see that the set of such ψ is compact in the $\|\cdot\|_1^{(5r_0)}$ norm. Thus, $Z(2r_0)(\mu + B)^{-1}$ is a compact operator, and so the hypotheses of Theorem XI.91 are satisfied.

The situation in this example has been studied in great detail and much more information is known. For example, $\mu \in \sigma(B)$ if and only if the reduced wave equation

$$\begin{aligned}
\Delta v - \mu^2 v &= 0 \\
v &= 0 \qquad \text{on } \partial D
\end{aligned} \tag{228}$$

has a solution v so that the data $\langle v, -\mu v\rangle$ is eventually outgoing, that is, satisfies $W_0(\rho)\langle v, -\mu v\rangle \in D_+$ for ρ large enough. The detailed relationship between these eigenvalues and the geometry of the obstacle has been the object of much study. Finally, the scattering operator $\hat{S}$ has the form (recall that $N = L^2(S^2)$)

$$\begin{aligned}(\hat{S}f)(\sigma, \omega) &= s(\sigma)f(\sigma, \omega)\\ &= f(\sigma, \omega) - \frac{i\sigma}{2\pi}\int_{|\theta|=1} \overline{k(\theta, \omega; \sigma)}\, f(\sigma, \theta)\, d\theta\end{aligned}$$

where $k(\theta, \omega; \sigma)$ is an analytic function of its variables which is related to the asymptotic behavior of the solutions of (228). This relationship is identical to the one between the quantum-mechanical T-matrix and the asymptotics of the solutions of the Lippmann–Schwinger equation.

It is clear from Examples 1, 2, and 4 that the Lax–Phillips method applies most naturally to classical wave equations where one has Huygens' principle, that is, in odd dimensions greater than one. Nevertheless, the theory can be applied in a variety of other situations as well (see the Notes for references).

Example 5 (application to the Schrödinger equation) As a last example we shall discuss how one can use the Lax–Phillips theory to study scattering for

$$i\,\frac{\partial u}{\partial t} = (-\Delta + V)u$$

The basic idea is to use the invariance principle for wave operators for the wave operators of the classical system

$$\begin{gathered} u_{tt} - \Delta u + V(x)u = 0 \\ u(x, 0) = f(x), \qquad u_t(x, 0) = g(x) \end{gathered} \tag{229}$$

We shall not obtain any results on the quantum-mechanical scattering operator that we have not already obtained in greater generality in Sections 4, 6, and 7, but it is interesting to get the results in a new way. We also emphasize that we shall need detailed spectral information about $-\Delta + V$ in order to apply the Lax–Phillips theory.

Let $V(x)$ be a potential with compact support in $\mathbb{R}^3$ and suppose that $V(x) \in L^2(\mathbb{R}^3)$ and $V(x) \geq 0$. First we want to solve (229). This is done analogously to the case of an inhomogeneous medium. Since $V \in L^2$, V is $-\Delta$-bounded (see Theorem X.15) so $-\Delta + V(x)$ is essentially self-adjoint. Further

$$((-\Delta + V)h, h) \geq (-\Delta h, h) \geq 0$$

so if $B_1 = \sqrt{-\Delta + V}$, we have $\|B_1 h\|_2 \geq \|B_0 h\|_2$. Moreover, $\mathscr{H}_1 \equiv [D(B_1)] \oplus L^2(\mathbb{R}^3) = \mathscr{H}_0$ since $-\Delta$ and $-\Delta + V$ have equal form domains. As before, if we define $W_1(t) = e^{-iA_1 t}$ where

$$A_1 = i\begin{pmatrix} 0 & I \\ -B_1^2 & 0 \end{pmatrix}$$

then the first component of $W_1(t)\langle f, g\rangle$ is a weak solution of (229) and a classical solution if f, g, and V are smooth enough.

The verification of hypotheses (i)–(iii) is analogous to Examples 2 and 4. Choose r_0 so that the ball $B(r_0)$ contains the support of $V(x)$ in its interior. Define $J: \mathscr{H}_0 \to \mathscr{H}_1$ to be the identity on those $\varphi \in \mathscr{H}_0$ with support outside $B(r_0)$ and any bounded injection on the orthogonal complement of this set. Finally, we take $D_+^{r_0}$ and $D_-^{r_0}$ to be $W_0(r_0)D_+$ and $W_0(-r_0)D_-$. As in the previous examples, properties (i) and (ii) for $U_1(t)$ and the orthogonality of $D_+^{r_0}$ and $D_-^{r_0}$ just follow from the corresponding properties of $W_0(t)$. Thus, if we can prove (iii), then we have verified the hypotheses of Theorem XI.86. To prove (iii) notice that the solutions of (229) propagate at speed one, so Lemmas 1 and 2 of Example 2 go through as before and the local compactness result of Lemma 3 is the same. Therefore, we need only show that $-\Delta + V$ has only absolutely continuous spectrum, and this is done by appealing to the same theorems that we appealed to in Example 2. Thus, by Theorem XI.82, we have the Lax–Phillips scattering operators S, $\tilde{S}$, and $\hat{S}$. By Theorem XI.86, $\Omega^{\pm}$ exist, are complete, and (215) holds.

An argument similar to that in Example 4 shows that $Z(2r_0)(\mu + B)^{-1}$ is compact for $\operatorname{Re}\mu > 0$ where $Z(t) = P_+ W_1(t) P_-$ and B is its generator. Thus $(\hat{S}f)(\sigma) = s(\sigma)f(\sigma)$ for all $f \in L^2(\mathbb{R}; S^2)$ where $s(\sigma)$ is meromorphic in the whole plane (with poles as singularities) and analytic on the real axis and in the upper half-plane.

Notice that for all data $\varphi \in C_0^\infty(\mathbb{R}^3) \times C_0^\infty(\mathbb{R}^3)$ and $|t|$ sufficiently large,

$$W_1(-t)JW_0(t)\varphi = W_1(-t)W_0(t)\varphi$$

and is independent of t. Just as in Examples 2 and 4, this follows because $W_0(t)$ satisfies Huygens' principle. Using Theorem XI.23, we conclude that the strong limits

$$\Omega^{\pm} = \operatorname*{s-lim}_{t \to \mp\infty} e^{+iA_1{}^2 t} e^{-iA_0{}^2 t}$$

exist and equal the wave operators already defined when applied to functions $\varphi \in E_{[0,\infty)}(A_0)$. But

$$A_0^2 = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix}$$

and

$$A_1^2 = \begin{pmatrix} -\Delta + V & 0 \\ 0 & -\Delta + V \end{pmatrix}$$

Thus

$$\Omega^\pm = \begin{pmatrix} \Omega_S^\pm(-\Delta + V, -\Delta) & 0 \\ 0 & \Omega_S^\pm(-\Delta + V, -\Delta) \end{pmatrix}$$

Therefore, the Schrödinger wave operators exist and are complete.

Further development shows that the fibers of the Schrödinger S-operator are given by

$$e^{-i2r_0E}s(\sqrt{E})$$

where $s(\cdot)$ are the $\mathscr{L}(L^2(S^2))$ fibers of the Lax–Phillips operator $\tilde{S}$. From the properties of $s(\cdot)$ discussed above it follows that $e^{i2r_0E}s(\sqrt{E})$ is meromorphic on a two-sheeted Riemann surface, analytic on the "physical" sheet with poles on the "unphysical sheet."

Before concluding this example, it is worthwhile to make several remarks. First, notice that we needed quite a bit of sophisticated information about the interacting system, namely the character of $\sigma(-\Delta + V)$ in order to use the Lax–Phillips approach. Secondly, we have handled only the case $V \in L^2$, $V \geq 0$, and V has compact support. The restriction $V \in L^2$ is not serious. The second restriction can be avoided by a generalization of the ideas above. The reason we needed $V \geq 0$ was so that we could take the square root of $-\Delta + V$. But if $V \in L^2$ with compact support, then $-\Delta + V$ has at most finitely many negative eigenvalues (Theorem XIII.6) and on the complement of the space spanned by their eigenfunctions, $-\Delta + V$ will be nonnegative. One can then push through the technique of this example and one finds, as expected, that $e^{-i2r_0E}s(\sqrt{E})$ has additional poles on the physical sheet at precisely the negative eigenvalues. The third restriction, that V have compact support, is much more serious since no potential in nature is believed to have compact support. And, it is crucial to all we have done in this section that the free and interacting systems are *identical* outside a bounded region.

Appendix to Section XI.11: The twisting trick

In this appendix we want to show that the Dirichlet Laplacian, $H_{D;\Gamma}$, exterior to a bounded region has empty singular continuous spectrum. We shall use a method (the twisting trick) which is applicable in a variety of other situations; see the reference in the Notes.

Theorem XI.91.5 Let Γ be a closed bounded set in $\mathbb{R}^n$ so that $\mathbb{R}^n\backslash\Gamma$ is connected. Let $H_{D;\Gamma}$ be the Dirichlet Laplacian defined in Section XIII.15. Fix $a > 0$. Let $X_a^{(\Gamma)}$ be the Hilbert space of functions $f \in L^2(\mathbb{R}^n\backslash\Gamma)$ with $e^{a|x|}f \in L^2$. Then, there is a set, $\mathscr{E}$, discrete in $\mathbb{R}\backslash\{0\}$, and a neighborhood N of $\mathbb{R}$ so that $(H_{D;\Gamma} - k^2)^{-1}$ can be extended as an analytic $\mathscr{L}(X_a^{(\Gamma)}, X_{-a}^{(\Gamma)})$-valued function from the region $\{k \mid \operatorname{Im} k > 0\}$ to $N\backslash\mathscr{E}$. In particular, $H_{D;\Gamma}$ has purely absolutely continuous spectrum.

Proof Since $\mathbb{R}^n\backslash\Gamma$ is connected, $H_{D;\Gamma}$ has no positive eigenvalues by the argument in Theorem XIII.56 (see especially the discussion preceding Theorem XIII.57). By Theorem XIII.20, the assertion about $\mathscr{L}(X_a^{(\Gamma)}, X_{-a}^{(\Gamma)})$ analyticity in $N\backslash\mathscr{E}$ shows that $\sigma_{\text{sing}}(H_{D;\Gamma}) = \varnothing$ since we can take X_a to be the dense set D and $[a, b]$ to be any closed interval disjoint from $\mathscr{E}$. Since $H_{D;\Gamma} \geq 0$ with empty kernel, $H_{D;\Gamma}$ clearly has no nonpositive eigenvalues. Thus, if we can prove the X_a assertion we will have a proof that the spectrum is purely absolutely continuous.

Define the operator H_α on $\mathscr{H} = L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n\backslash\Gamma)$ by

$$H_\alpha\langle\varphi, \psi\rangle = \langle(-\Delta + \alpha x^2)\varphi, H_{D;\Gamma}\psi\rangle$$

Suppose that $(H_\alpha - k^2)^{-1}$ has an $\mathscr{L}(X_a \oplus X_a^{(\Gamma)}, X_{-a} \oplus X_{-a}^{(\Gamma)})$ continuation onto $N_\alpha\backslash\mathscr{E}_\alpha$ where each $\mathscr{E}_\alpha$ may have some finite accumulation points but so that for any $\varepsilon > 0$ and $a > 0$, we can find an α so that $[\mathscr{E}_\alpha \cap (-a, a)]\backslash(-\varepsilon, \varepsilon)$ is a finite set. Then the result follows easily.

Define a "twisting operator" U on $\mathscr{H}$ as follows. Choose R so that $\Gamma \subset \{x \mid |x| < R\}$ and choose a C^∞, 2 × 2 unitary-matrix-valued function on $\mathbb{R}^n$, $u(x)$, so that

$$u(x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{if} \quad |x| > 2R$$

$$u(x) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{if} \quad |x| < R$$

Define $(U\psi)(x) = u(x)\psi(x)$. Then U is unitary on $\mathscr{H}$ and on $X_{\pm a} \oplus X_{\pm a}^{(\Gamma)}$, so it suffices to prove the claimed continuation property for $UH_\alpha U^{-1}$. But $\tilde{H}_\alpha \equiv UH_\alpha U^{-1} = T_\alpha + V_\alpha$ where

$$T_\alpha\langle\varphi, \psi\rangle = \langle -\Delta\varphi, (H_{D;\Gamma} + \alpha x^2)\psi\rangle$$

$$V_\alpha = f_\alpha \cdot p + g_\alpha$$

where $p = i^{-1}\nabla$ and f_α and g_α are 2 × 2 matrices of C_0^∞ functions. Let $S_\alpha = \sigma(H_{D;\Gamma} + \alpha x^2)$ which is discrete (see Section XIII.14). By the analysis in the appendix to Section XI.6 (see especially Theorem XI.45), $(\tilde{H}_\alpha - k^2)^{-1}$

has an $\mathscr{L}(X_a, X_{-a})$ continuation to $N_\alpha \backslash \mathscr{E}_\alpha$ where the only possible limit points of N_α lie in $S_\alpha \cup \{0\}$, because $(T_\alpha - k^2)^{-1}$ has such a continuation on $\{k \mid \operatorname{Im} k > -a,\ \arg k \neq -\pi/2\} \backslash S_\alpha$. But $\inf S_\alpha \geq \inf(-\Delta + \alpha x^2)$ goes to infinity as $\alpha \to \infty$, so we can pick α so that $[\mathscr{E}_\alpha \cap (-a, a)] \backslash (-\varepsilon, \varepsilon)$ is finite. ▮

XI.12 The linear Boltzmann equation

In this section we describe a mathematical model for the scattering of a low-density beam of neutrons off a chunk of material such as uranium in free space. This model has only limited physical interest since it does not cover the nonscattering case where the number of neutrons grows exponentially in time, that is, the uranium blows up, nor the case where the neutron beam is constrained by shielding to stay in a bounded region filled with uranium and graphite rods, that is, a reactor. However, the model we describe is mathematically quite interesting since it provides a situation where the Hilbert space scattering theory must be extended in two ways: In the first place, the natural space of states is not a Hilbert space but a cone in a (non-Hilbert) vector space; in the second place, the equation of motion we describe defines a one-sided dynamics since the quantum aspects of the problem are modeled on a classical level by using statistical ideas. Moreover, the theory illustrates the natural use of semigroups on a Banach space.

The basic dynamical object is a positive function $n(x, v)$ on $\mathbb{R}^3 \times \mathbb{R}^3$ representing the density of neutrons at a point $\langle x, v \rangle$ in phase space. For a suitable integer N_0,

$$N_0 \int_{A \times B} n(x, v)\, d^3x\, d^3v$$

represents the number of neutrons in the set A with velocities in the set B. Of course, if $n(x, v)$ is a function, the number cannot be integral for all A and B; put differently, $n(x, v)$ should really be $N_0^{-1} \sum_{i=1}^{N_0} \delta(x - x_i)\, \delta(v - v_i)$. But if N_0 is large (it is typically at least 10^{20} for realistic experiments), it is a reasonable approximation to take $n(x, v)$ as an L^1 function. Thus, it is natural to take L_+^1, the cone of *positive* functions on $\mathbb{R}^3 \times \mathbb{R}^3$, as the set states of the system.

The dynamical equation postulated for $n(x, v)$ is

$$\frac{d}{dt} n(x, v, t) = -v \cdot \nabla_x n(x, v, t) + \int k(x, v', v) n(x, v', t)\, dv' - \sigma_a(x, v) n(x, v, t) \tag{230}$$

which is called the **linear Boltzmann equation.** To understand its meaning, let us solve the equation when k and σ_a are zero. Let

$$[W_0(t)n](x, v) = n(x - vt, v) \tag{231}$$

Theorem XI.92 For each $p \in [1, \infty]$ and in particular for $p = 1$, $W_0(t)$ is a strongly continuous group of isometries on $L^p(\mathbb{R}^6)$ taking positive functions into positive functions. Moreover, on each L^p, $p < \infty$, $C_0^\infty(\mathbb{R}^6)$ is a core for the infinitesimal generator of $W_0(t)$ and $W_0(t) = e^{-tT_0}$ where

$$T_0 f = v \cdot \nabla_x f \tag{232}$$

for $f \in C_0^\infty$.

Proof All the statements follow immediately from (231) except for the core statement and (232). These follow from Theorem X.49 if one notices that, by (231), C_0^∞ is left invariant by $W_0(t)$, that $W_0(t)f$ is C^∞ in t for $f \in C_0^\infty$, and that

$$-\frac{d}{dt} W_0(t)f \bigg|_{t=0} = v \cdot \nabla_x f \quad \blacksquare$$

Thus, the first term on the right-hand side of the linear Boltzmann equation (230) describes the free classical motion of a group of neutrons with no scattering, no absorption, and no production. The second term has a very simple interpretation. A neutron at point $\langle x, v' \rangle$ in phase space may, due to scattering or to some production process such as fission, become or produce a neutron with a different velocity v. The total rate of production by or scattering from a neutron at $\langle x, v' \rangle$ is given by

$$\sigma_p(x, v') = \int k(x, v', v)\, dv \tag{233}$$

Similarly, the last term on the right-hand side of (230) represents the loss of neutrons from a point $\langle x, v \rangle$ in phase space due to scattering into other points $\langle x, v' \rangle$ in phase space or due to absorbtion (for example, by graphite rods).

Throughout our discussion we shall make the following assumptions on k, σ_a, and σ_p.

Definition We say that the pair $\langle k, \sigma_a \rangle$ is **regular** if and only if:

(i) k is a nonnegative measurable function on $\mathbb{R}^9$ and σ_a is a nonnegative measurable function on $\mathbb{R}^6$.

(ii) For each $\langle x, v' \rangle$, $k(x, v', \cdot)$ is in L^1 and σ_a and σ_p are uniformly bounded functions on $\mathbb{R}^6$.

(iii) There is a compact set D in $\mathbb{R}^3$ so that $k(x, v, v')$ and $\sigma_a(x, v)$ vanish if $x \notin D$.

Before studying solutions and scattering theory for (230), we would like to make several comments about the form of the equation and about our assumptions of "regularity." (230) has a "probabilistic" or "statistical" nature in that we are interpreting the latter two terms in terms of a certain fraction of the particles at $\langle x, v\rangle$ being produced, scattered, or absorbed. One can understand this statistical element as entering from one of two sources: In the first place, even classically the positions of the uranium atoms are changing due to thermal motions; secondly, since at its base the scattering is quantum mechanical, it is intrinsically given by probabilities. While one can easily understand the probabilistic nature of the equation (230), it has some surprising consequences. For example, despite the fact that we are thinking of the equation as describing the motion of an aggregation of particles, each obeying a particle dynamics that is given by time reversible laws (Newton's equation), the equation (230), *as an equation on* L^1_+, is only solvable for positive times, as we shall see below.

The reason that the term "linear" is added to the name is that the original equations proposed by Boltzmann (to describe gases, not neutrons) contained a quadratic term in n due to the scattering of the basic particles off one another. In the "small" n limit this term is unimportant. Physically, "small" n means that the density of neutrons is low compared to the density of scattering objects and low enough so that it is unlikely that two neutrons get close enough to interact significantly. These assumptions are not unreasonable.

The assumption that σ_a and σ_p have bounded supports in the x variable is not really necessary for the mathematical theory although it is natural from a physical point of view. See the Notes for a reference that describes the scattering theory if σ_a and σ_p are only assumed to fall off sufficiently rapidly. We remark that σ does not stand for a cross section but for a rate.

There are three situations that have obvious physical interpretations. The first is where $\sigma_a(x, v) = \sigma_p(x, v)$ for all $x, v \in \mathbb{R}^6$. Here the number of neutrons that leave $\langle x, v\rangle$ is precisely equal to the number of neutrons that enter other regions of phase space due to the presence of neutrons at $\langle x, v\rangle$. For obvious reasons, this is called the **pure scattering case**. Similarly $\sigma_a \leq \sigma_p$ is called the **production case** and $\sigma_a \geq \sigma_p$ the **absorption case**.

Finally, we remark on the apparent lack of conservation of energy in (230). For we do not require k to be supported in the region where $|v| = |v'|$; in fact, since k is a function rather than a distribution or measure, k cannot be supported in that region without being zero almost everywhere.

One can develop the theory by replacing

$$\int k(x, v', v)n(x, v', t)\, dv' \qquad \text{by} \qquad \int k(x, |v|\Omega', v)n(x, |v|\Omega', t)\, d\Omega'$$

and this is appropriate in some ways in the pure scattering case. But there is a physical reason why a spread of final velocities is appropriate. For the uranium nuclei are not fixed, so the final velocity is dependent on the initial velocity of the uranium nuclei, even in elastic collisions. Since we "average" over positions of uranium nuclei in the statistical sense mentioned above, it is not unreasonable to "average" over velocities too.

Solving (230) is an exercise in the theory of semigroups on Banach spaces:

Theorem XI.93 Let $\langle k, \sigma_a \rangle$ be a regular pair. Then there exists a one-parameter strongly continuous semigroup $W(t)$, $t \geq 0$, on $L^1(\mathbb{R}^6)$ taking $L^1_+(\mathbb{R}^6)$ into itself, so that $W(t) = e^{-tT}$, with $C_0^\infty(\mathbb{R}^6)$ a core for T, and

$$Tf(x, v) = T_0 f(x, v) - \int k(x, v', v) f(x, v')\, dv' + \sigma_a(x, v) f(x, v)$$

Moreover:

(a) $D(T) = D(T_0)$.
(b) $\|W(t)\| \leq e^{Ct}$ with $C = \|\sigma_p\|_\infty$.
(c) In the pure scattering (respectively, absorption) case $\|W(t)n\|_1 = \|n\|_1$ (respectively, $\|W(t)n\|_1 \leq \|n\|_1$) for all $n \in L^1_+$.
(d) For any $n \in L^1_+$ and all $\langle x, v \rangle$ and $t > 0$,

$$[W(t)n](x, v) \geq n(x - tv, v) \exp\left(-\int_0^t \sigma_a(x - sv, v)\, ds\right) \tag{234}$$

Proof Define operators A_1, A_2 on $L^1(\mathbb{R}^6)$ by

$$(A_1 n)(x, v) = -\int k(x, v', v) n(x, v')\, dv'$$

$$(A_2 n)(x, v) = \sigma_a(x, v) n(x, v)$$

Then A_1 and A_2 are bounded with norms $\|\sigma_p\|_\infty$ and $\|\sigma_a\|_\infty$, respectively. Moreover, if $\tilde{T} = T_0 + A_2$, then $\tilde{W}(t) = e^{-t\tilde{T}}$ is given by the explicit formula

$$(\tilde{W}(t)n)(x, v) = n(x - tv, v) \exp\left(-\int_0^t \sigma_a(x - sv, v)\, ds\right) \tag{235}$$

Since $T = T_0 + A_1 + A_2$, it follows from Theorem X.50 that T generates an exponentially bounded semigroup, that any core for T_0 is one for T, and that $D(T) = D(T_0)$. Since $\|e^{-tA_1}\| \le e^{t\|A_1\|}$ and $\|\tilde{W}(t)\| \le 1$, it follows from the Trotter product formula (Theorem X.51) that

$$\|W(t)\| \le \|e^{-tA_1}\| \le \exp(t\|\sigma_{\mathrm{p}}\|_\infty)$$

proving (b).

As in Section X.9 (step 4 in the proof of Theorem X.58), one verifies Duhamel's formulas:

$$W(t) = W_0(t) - \int_0^t W_0(t-s)(A_1 + A_2)W(s)\,ds \tag{236}$$

and

$$W(t) = \tilde{W}(t) - \int_0^t W(t-s)A_1\tilde{W}(s)\,ds \tag{237}$$

Now e^{-A_1t} is positivity preserving since $-A_1$ is and one can expand the exponential. Thus, by the Trotter product formula, and the fact $\tilde{W}$ is obviously positivity preserving, we conclude that $W(t)$ takes L_+^1 into itself. Moreover, by (237) $W(t)n \ge \tilde{W}(t)n$ pointwise, which proves (234).

All that remains is part (c). Notice that

$$\int [W_0(t)n](x, v)\,dx\,dv = \int n(x, v)\,dx\,dv$$

$$\int (A_1n)(x, v)\,dx\,dv = -\int \sigma_{\mathrm{p}}(x, v')n(x, v')\,dx\,dv'$$

so, by (236) and properties of $W_0(t)$,

$$\int (W(t)n)(x, v)\,dx\,dv$$

$$= \int n(x, v)\,dx\,dv + \int_0^t ds \int [\sigma_{\mathrm{p}}(x, v) - \sigma_{\mathrm{a}}(x, v)](W(s)n)(x, v)\,dx\,dv \tag{238}$$

from which (c) follows immediately. ▌

We are now in a position to explain the sense in which the dynamical operator $W(t)$ is not invertible. As a map from L^1 to L^1 it is invertible since $-T_0 - A_1 - A_2$ generates a semigroup, but this inverse does not in general take L_+^1, the basic set of states, into itself; for an example of this phenomenon see the reference in the Notes. Given a one-sided dynamics $W(t)$

($t \geq 0$) and a two-sided comparison dynamics $W_0(t)$ ($-\infty < t < \infty$), it is fairly obvious that the natural scattering theory objects are

$$\Omega^+ = \operatorname*{s-lim}_{t \to -\infty} W(-t)W_0(t) \tag{239}$$

$$\tilde{\Omega}^- = \operatorname*{s-lim}_{t \to +\infty} W_0(-t)W(t) \tag{240}$$

$\Omega^+ n_0$ is the value at $t = 0$ of the solution of the interacting problem, which looks like $W_0(t)n_0$ in the distant past. And $\tilde{\Omega}^- n_1$ is the value at $t = 0$ for the free propagation, which looks more and more like $W(t)n_1$ as $t \to +\infty$. Thus, if Ω^+ and $\tilde{\Omega}^-$ exist, the scattering operator is given by

$$S = \tilde{\Omega}^- \Omega^+$$

Notice that (239) and (240) involve $W(t)$ only for t positive. On the basis of the examples we have previously discussed, we expect the existence of the limit (239) to be easier than that of (240).

Further, there are cases where one does not expect either of them to exist. For, if there is too much neutron production, the number of neutrons may grow indefinitely with time, in which case physically the uranium blows up and mathematically we are in a nonscattering situation. We therefore single out a class of interactions.

Definition We say that a regular pair $\langle k, \sigma_a \rangle$ is **subcritical** if and only if $\sup_{t \geq 0} \|W(t)\| < \infty$.

By (238), $\langle k, \sigma_a \rangle$ is subcritical in the pure scattering and absorbtive cases. We shall see below (Theorem XI.95) that it is also subcritical in the production case if the chunk of matter is sufficiently small.

The following simple geometric lemma is crucial both in controlling the limit (239) and in proving subcriticality in the small region production case. Intuitively, it says that the number of neutrons in a bounded region goes down quite fast as long as there are not too many with very small velocities to begin with.

Lemma For any Borel set $D \subset \mathbb{R}^3$, let $\|n\|_D = \int_{x \in D} \int_{\mathbb{R}^3} n(x, v)\, dx\, dv$. Then for $n \in L^1_+(\mathbb{R}^6)$

$$\int_{-\infty}^{\infty} \|W_0(t)n\|_D \, dt \leq (\operatorname{diam} D) \|v^{-1} n\|_{L^1(\mathbb{R}^6)}$$

where $\operatorname{diam} D = \sup_{x, y \in D} |x - y|$.

Proof It suffices to prove that for each fixed $v \neq 0$,

$$\int_{-\infty}^{\infty} \int_{x \in D} |W_0(t)n(x, v)| \, dx \, dt \leq [\text{diam } D] \int |v|^{-1} |n(x, v)| \, dx \tag{241}$$

Let χ be characteristic function of D. Then the left-hand side of (241) is $\int_{-\infty}^{\infty} (\int \chi(x) |n(x - vt, v)| \, dx) \, dt$. Let y be the component of x parallel to v and $x_\perp$ the two coordinates orthogonal. Then the last integral can be written

$$\begin{aligned} &\int_{-\infty}^{\infty} dt \int dx_\perp \int dy \, \chi(y, x_\perp) |n(y - |v|t, x_\perp, v)| \\ &\qquad = |v|^{-1} \int dz \int dx_\perp \int dy \, \chi(y, x_\perp) |n(z, x_\perp, v)| \\ &\qquad \leq |v|^{-1} (\text{diam } D) \iint dx_\perp \, dz \, |n(z, x_\perp, v)| \end{aligned}$$

proving (241). In the above, we changed variables from t to $z = y - |v|t$ in the first step and used the obvious geometric fact $|\int \chi(y, x_\perp) \, dy| \leq \text{diam } D$ in the second. ▮

Theorem XI.94 If $\langle k, \sigma_a \rangle$ is a regular pair defining a subcritical system, then Ω^+ exists and is a positivity preserving operator. Ω^+ is a contraction (respectively, isometry) in the absorbtion (respectively, pure scattering) case.

Proof Since $\langle k, \sigma_a \rangle$ is subcritical, the family $\{W(-t)W_0(t)\}$ is uniformly bounded. Thus, it suffices to prove that the limit (239) exists for a dense set $\mathscr{D}$ in L^1. The other properties of Ω^+ follow from those of $W(-t)$ and $W_0(t)$. Take

$$\mathscr{D} = \left\{ n \in C_0^\infty(\mathbb{R}^6) \,\middle|\, |v|^{-1} n \in L^1 \right\}$$

Let $A = A_1 + A_2$ as in Theorem XI.93 and let D be a bounded set containing supp σ_a and supp σ_p. Then for $n \in \mathscr{D}$,

$$\begin{aligned} \int_{-\infty}^{0} \|A W_0(t) n\| \, dt &\leq \|A\| \int_{-\infty}^{0} \|W_0(t) n\|_D \, dt \\ &\leq \|A\| (\text{diam } D) \|v^{-1} n\|_1 < \infty \end{aligned}$$

by the lemma. By Cook's method, the limit (239) exists. ▮

We need a further condition on $\langle k, \sigma_a \rangle$ to make the interaction subcritical if the volume of matter is small. We say that $\langle k, \sigma_a \rangle$ has **finite mean free path** if

$$M(\sigma_p) \equiv \|v^{-1}\sigma_p\|_\infty < \infty$$

The reason for the name is that $(v^{-1}\sigma_p)^{-1}$ represents a distance between successive collisions or particle productions.

Theorem XI.95 A regular pair $\langle k, \sigma_a \rangle$ with finite mean free path that obeys $(\text{diam } D)M(\sigma_p) < 1$ is subcritical and, in particular, Ω^+ exists.

Proof Using (237) and the fact that $\tilde{W}(t)$ is a contraction, we easily obtain

$$\sup_{0 \le t \le T} \|W(t)\| \le 1 + \alpha \sup_{0 \le t \le T} \|W(t)\|$$

where

$$\alpha \equiv \int_0^\infty \|A_1 \tilde{W}(s)\| \, ds$$

Thus, if $\alpha < 1$,

$$\sup_{0 \le t < \infty} \|W(t)\| \le (1 - \alpha)^{-1}$$

and the system is subcritical. Therefore, we need only prove that

$$\alpha \le (\text{diam } D)M(\sigma_p) \tag{242}$$

Since $\|A_1 v^{-1}\|_{\text{op}} = M(\sigma_p)$, (242) follows if we prove that

$$\int_0^\infty \|v\tilde{W}(s)n\|_D \, ds \le (\text{diam } D)\|n\|_1$$

But v commutes with $\tilde{W}(s)$ and $\|\tilde{W}(s)n\|_D \le \|W_0(s)n\|_D$, so, by the lemma,

$$\int_0^\infty \|v\tilde{W}(s)n\|_D \, ds \le (\text{diam } D)\|vv^{-1}n\|_1$$

This proves (242) and thus the theorem. ▌

Basically, the condition $\alpha < 1$ in the proof implies that the iteration of (237) converges uniformly in t. The physical reason for this is that $(\text{diam } D)M(\sigma_p) < 1$ says that, to first order, a particle passing through D undergoes less than one collision and so the geometric series obtained by iterating and using $\alpha < 1$ converges. We note that Theorem XI.95 provides us with a large variety of semigroups bounded in time which are not contraction semigroups. With one more condition we can now prove the existence of the limit (240).

Theorem XI.96 Suppose that the system defined by the regular pair $\langle k, \sigma_a \rangle$ has finite mean free path, is subcritical, and that

$$M(\sigma_a) \equiv \|v^{-1}\sigma_a\|_\infty < \infty$$

Then $\tilde{\Omega}^-$ exists. The scattering operator $S = \tilde{\Omega}^-\Omega^+$ is a bounded one-to-one map of $L^1_+(\mathbb{R}^6)$ into itself.

Proof Let $\sigma_1 = \sigma_p$ and $\sigma_2 = \sigma_a$. We first claim that for all $\langle x, v \rangle \in \mathbb{R}^6$,

$$\int_0^\infty \sigma_i(x - sv, v)\, ds \le [\text{diam } D] M(\sigma_i) \tag{243}$$

(243) is proven just as in the proof of the lemma. By (d) of Theorem XI.93 and (243),

$$(W(t)n)(x, v) \ge \exp(-[\text{diam } D]M(\sigma_2))n(x - vt, v)$$

for n positive. Letting $C = \exp([\text{diam } D]M(\sigma_2))$, we have

$$n(x, v) \le C(W(t)n)(x + vt, v) \tag{244}$$

Thus, replacing n by $W(s)n$ and t by $t - s$,

$$(W(s)n)(x, v) \le C(W(t)n)(x + v(t - s), v)$$

Therefore, for n positive,

$$\begin{aligned}
\int_0^t \|A_i W(s)n\|_1\, ds &= \int_0^t ds \int \sigma_i(x, v)(W(s)n)(x, v)\, dx\, dv \\
&\le C \int_0^t ds \int \sigma_i(x, v)(W(t)n)(x + v(t - s), v)\, dx\, dv \\
&= C\left(\int_0^t \sigma_i(y - vr, v)\, dr\right) \int (W(t)n)(y, v)\, dy\, dv \\
&\le C(\text{diam } D)M(\sigma_i)\|W(t)n\|_1
\end{aligned}$$

In the next to last step we changed variables in two places and in the last step used (243). It follows that

$$\int_0^\infty \|A_i W(s)n\|_1\, ds \le C[\text{diam } D]M(\sigma_i) \sup_{t \ge 0} \|W(t)n\|_1$$

As a result, subcriticality implies that

$$\int_0^\infty \|A_i W(s)n\|_1 \, ds < \infty$$

which by Cook's method implies the existence of the limit (240). Ω^+ exists by Theorem XI.94; and since $\{W(t)\}$ is uniformly bounded and each $W(t)$ is positivity-preserving, Ω^+, $\tilde{\Omega}^-$ are bounded positivity-preserving operators on $L_+^1(\mathbb{R}^6)$. Therefore, the same is true of $S = \tilde{\Omega}^-\Omega^+$. By (244)

$$\|W(t)n\|_1 \geq C^{-1}\|n\|_1$$

for n positive. From this and the fact that $W_0(t)$ is an isometry it easily follows that S is one-to-one. ▌

XI.13 Nonlinear wave equations

...formerly unsolvable equations are dealt with by threats of reprisals. *Woody Allen*

In this section we give an introduction to the scattering theory of nonlinear classical wave equations. There are many unsolved problems in this area, and the scattering theories that do exist are typically valid only for special nonlinear terms. The general ideas follow the outline given in Section 1, although the techniques for proving estimates are more difficult than in the linear case. Let us begin by looking at the equation

$$u_{tt} - \Delta u + m^2 u = F(u) \tag{245}$$

In Section X.13 we developed the existence theory for (245) for the case $F(u) = \pm\lambda|u|^{p-1}u$, where $p = 3$. The same method works for $p < 5$. To develop a scattering theory for (245) one might try to show that for large positive and negative times, its solutions look more and more like solutions of the corresponding free equation:

$$u_{tt} - \Delta u + m^2 u = 0 \tag{246}$$

The solutions of this free equation with nice initial data decay in the sup norm like $t^{-n/2}$ in n space dimensions (see Theorem XI.17). If the same decay holds for solutions of (245), a scattering theory should exist since a term like $-\lambda|u|^{p-1}u$ will decay faster than the linear terms if $p > 1$. However, even for the linear Schrödinger equation, one does not expect all solutions of the interacting equation to decay since there may be bound states. There should also be bound states for (245), at least for suitable F.

Suppose that F has the form $F(y) = yH(|y|)$ where $H(|y|) \to 0$ as $|y| \to 0$. Then (245) has a solution of the form

$$u_0(x, t) = e^{i\omega t}\varphi(x) \tag{247}$$

if and only if

$$-\Delta\varphi(x) + V(x)\varphi(x) = -(m^2 - \omega^2)\varphi(x) \tag{248a}$$

$$V(x) = -H(|\varphi(x)|) \tag{248b}$$

Except for very pathological potentials, the Schrödinger equation will not have positive eigenvalues (see Section XIII.13). Thus, we restrict our attention to the case $|\omega| < m$. If $V(x)$ is positive, for example if $F(u) = -\lambda u|u|^2$, then of course (248a) will have no such solutions since $-\Delta + V \geq 0$. If $V(x)$ is not always positive, then it is not surprising that solutions exist. In fact, the reference given in the Notes constructs large classes of F's with solutions of (248). An explicit example where such solutions exist is

$$F(u) = -u(|u|^2 - \lambda|u|)$$

for suitably large λ.

If solutions of the form (247) exist, then there should be solutions of (245) which look asymptotically (as $t \to -\infty$) like $u_0(x, t)$ plus a solution of (246). Since the nonlinearity couples the bound state to the asymptotically free piece, there is no reason to expect that the bound state will be present as $t \to +\infty$. Thus, if there are bound states, the scattering theory for (245) is intrinsically a multichannel problem. In fact, there should be an infinite number of channels. For, by the Lorentz invariance of (245), the existence of a u_0 implies the existence of a solution of (245) of the form

$$\exp(i(t - v^{-1}x)\omega(v))\psi(x - vt)$$

Thus it should be possible to construct solutions of (245) that consist of n bumps moving relative to one another. In addition to this there are examples with infinitely many bound states for fixed ω. And, one expects bound states for every sufficiently small ω.

Thus, not only is the problem nonlinear, but the full complexity of multichannel scattering is present. The two general cases where asymptotic completeness can be proven are precise analogues of the two cases where asymptotic completeness has been known for multichannel Schrödinger systems for many years. The small data case which we present first is the analogue of weak coupling (Theorem XIII.27). The result discussed at the end of the section is the analogue of the repulsive potential case (Theorem XIII.32). In the middle part of the section we present a general construction of the channel wave operators for the channel where u is asymptotically free.

It is also worth mentioning at the outset two technical difficulties that arise here but not in linear quantum-mechanical scattering. First, since the wave and scattering operators are nonlinear, in order to prove existence it is not sufficient to prove that they exist on a dense set and then extend by the B.L.T. theorem. Secondly, it is natural to take as scattering states the set of initial data Σ_{scat} for which the solutions of (246) decay appropriately at $\pm\infty$. Unfortunately, only sufficient conditions are known for such decay, so the norm on Σ_{scat} typically involves explicitly the large time behavior of the solution of the corresponding linear equation. This causes some technical complications.

In Section X.13 we showed that (245) can be reformulated as

$$\varphi'(t) = -iA\varphi(t) + J(\varphi(t)) \tag{249a}$$

where $J(\langle u, v\rangle) = \langle 0, F(u)\rangle$,

$$A = i\begin{pmatrix} 0 & I \\ \Delta - m^2 & 0 \end{pmatrix}$$

and $\varphi(t) = \langle u(\cdot, t),\ v(\cdot, t)\rangle$ is viewed as a function from $\mathbb{R}$ to $D((-\Delta + m^2)^{\frac{1}{2}}) \oplus L^2(\mathbb{R}^3)$. This led us to study the existence theory of (249a) as an abstract problem where $\varphi(t)$ takes values in a Hilbert space $\mathscr{H}$, A is self-adjoint on $\mathscr{H}$, and J is a nonlinear mapping of $\mathscr{H}$ into itself. Under the condition that J be uniformly Lipschitz on balls in $\mathscr{H}$ we proved that the corresponding integral equation

$$\varphi(t) = e^{-itA}\varphi_0 + \int_0^t e^{-iA(t-s)} J(\varphi(s))\, ds \tag{249b}$$

has a unique continuous $\mathscr{H}$-valued solution φ for small t. If J satisfies additional estimates and the initial data φ_0 are in $D(A)$, then we showed that φ is strongly differentiable and (249a) holds. In this section we shall always work with (249b); the reader should consult Section X.13 for the sufficient conditions that φ satisfy (249a).

We begin by presenting an abstract scattering theory for small data. Let A be a self-adjoint operator on $\mathscr{H}$. Let $\|\cdot\|_a$ and $\|\cdot\|_b$ be two auxiliary "norms" on $\mathscr{H}$: $\|\cdot\|_a$ satisfies all the properties of a norm except that $\|\varphi\|_a = 0$ need not imply that $\varphi = 0$; $\|\cdot\|_b$ satisfies all the properties of a norm except that it may take the value $+\infty$. We assume that A, J, and $\|\cdot\|_a$, $\|\cdot\|_b$ satisfy the following hypotheses:

(i) There is a $c > 0$ so that

$$\|\varphi\|_a \le c\|\varphi\| \qquad \text{for all} \quad \varphi \in \mathscr{H} \tag{250}$$

(ii) There are constants $c_1 > 0$, $d > 0$, so that for $\varphi \in \mathscr{H}$,

$$\|e^{-iAt}\varphi\|_a \le c_1 t^{-d}\|\varphi\|_b \qquad \text{if} \quad |t| \ge 1 \tag{251}$$

(iii) There exist $\beta > 0$, $\delta > 0$, and $q \ge 1$ with $dq > 1$, so that

$$\|J(\varphi_1) - J(\varphi_2)\| \le \beta(\|\varphi_1\|_a + \|\varphi_1\|_a)^q\|\varphi_1 - \varphi_2\| \tag{252}$$

$$\begin{aligned}\|J(\varphi_1) - J(\varphi_2)\|_b \le \beta\{(&\|\varphi_1\|_a + \|\varphi_2\|_a)^{q-1}\|\varphi_1 - \varphi_2\|_a \\ &+ (\|\varphi_1\|_a + \|\varphi_2\|_a)^q\|\varphi_1 - \varphi_2\|\}\end{aligned} \tag{253}$$

for all $\varphi_1, \varphi_2 \in \mathscr{H}$ satisfying $\|\varphi_i\| \le \delta$. In the case $q = 1$ we assume that β can be chosen arbitrarily small if δ is chosen small. Moreover, we assume that $J(0) = 0$.

We can now define the scattering states and the scattering norm. First, for an $\mathscr{H}$-valued function $\psi(t)$ on $\mathbb{R}$ we define

$$|||\psi(\cdot)|||_{[N_1, N_2]} \equiv \sup_{N_1 \le t \le N_2} \|\psi(t)\| + \sup_{N_1 \le t \le N_2} (1 + |t|)^d\|\psi(t)\|_a$$

In the case where $N_1 = -\infty$, $N_2 = +\infty$ we shall denote the norm simply by $|||\cdot|||$. Now we define

$$\Sigma_{\text{scat}} \equiv \left\{\varphi \in \mathscr{H} \,\middle|\, |||e^{-itA}\varphi||| < \infty\right\}$$

and

$$\|\varphi\|_{\text{scat}} \equiv |||e^{-itA}\varphi|||$$

That is, the scattering states are just those vectors in $\mathscr{H}$ that decay nicely in the $\|\cdot\|_a$ norm under the free propagation. Notice that if $\|\varphi\|_b < \infty$, then

$$\|e^{-itA}\varphi\|_a \le c_2(1 + |t|)^{-d}(\|\varphi\| + \|\varphi\|_b) \qquad \text{for all } t \tag{254}$$

so $\varphi \in \Sigma_{\text{scat}}$ and

$$\|\varphi\|_{\text{scat}} \le (1 + c_2)\|\varphi\| + c_2\|\varphi\|_b$$

Theorem XI.97 (global existence for small data) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J be a nonlinear mapping of $\mathscr{H}$ into itself. Suppose that there exist $\|\cdot\|_a$, $\|\cdot\|_b$ so that hypotheses (i)–(iii) hold. Then there is an $\eta_0 > 0$ so that for all $\varphi_- \in \Sigma_{\text{scat}}$ with $\|\varphi_-\|_{\text{scat}} \le \eta_0$, the equation

$$\varphi(t) = e^{-itA}\varphi_- + \int_{-\infty}^{t} e^{-iA(t-s)}J(\varphi(s))\,ds \tag{255}$$

has a unique global continuous $\mathscr{H}$-valued solution φ with $|||\varphi(\cdot)||| \le 2\eta_0$. Moreover:

(a) For each t, $\varphi(t) \in \Sigma_{\text{scat}}$.
(b) $\|\varphi(t) - e^{-itA}\varphi_-\| \to 0$ as $t \to -\infty$.

Proof The basic idea is to use the contraction mapping method which we employed in Section X.13 except with initial conditions at $t = -\infty$. Thus, this theorem is similar to our discussion in Section 2. Let X_{η, φ_-} denote the set of continuous $\mathscr{H}$-valued functions $\psi(t)$ so that $|||\psi(t) - e^{-itA}\varphi_-||| \le \eta$. Assume that $\|\varphi_-\|_{\text{scat}} \le \eta \le \frac{1}{2}\delta$ where δ is chosen so that hypothesis (iii) holds. For $\psi(\cdot) \in X_{\eta, \varphi_-}$, define

$$(\mathscr{J}\psi)(t) = \int_{-\infty}^{t} e^{-iA(t-s)}J(\psi(s))\, ds$$

As in the proof of Theorem X.72, it is easy to check that $e^{-iA(t-s)}J(\psi(s))$ is a continuous function of s for each t. Further, since $\|\psi(s)\| \le |||\psi(\cdot)||| \le |||e^{-itA}\varphi_-||| + \eta \le 2\eta$, we have

$$\begin{aligned}\|J(\psi(s))\| &\le \beta\|\psi(s)\|_a^q\|\psi(s)\| \\ &\le \beta|||\psi(\cdot)|||^{q+1}(1 + |s|)^{-dq} \\ &\le \beta(2\eta)^{q+1}(1 + |s|)^{-dq}\end{aligned}$$

by (252), so

$$\begin{aligned}\|(\mathscr{J}\psi)(t)\| &\le \int_{-\infty}^{t} \|e^{-iA(t-s)}J(\psi(s))\|\, ds \\ &\le \beta(2\eta)^{q+1}\int_{-\infty}^{t} (1 + |s|)^{-dq}\, ds < \infty \qquad (256)\end{aligned}$$

since $dq > 1$. Also

$$\begin{aligned}\|(\mathscr{J}\psi)(t)\|_a &\le \int_{-\infty}^{t} \|e^{-iA(t-s)}J(\psi(s))\|_a\, ds \\ &\le c_2\int_{-\infty}^{t} (1 + |t - s|)^{-d}(\|J(\psi(s))\|_b + \|J(\psi(s))\|)\, ds \quad \text{(by (254))} \\ &\le c_2\beta\int_{-\infty}^{t} (1 + |t - s|)^{-d}\{\|\psi(s)\|_a^q(1 + 2\|\psi(s)\|)\}\, ds \\ &\qquad\qquad \text{(by (252) and (253))} \\ &\le c_2\beta(2\eta)^q(1 + 4\eta)\int_{-\infty}^{t} (1 + |t - s|)^{-d}(1 + |s|)^{-dq}\, ds \qquad (257) \\ &\le c_2\beta(2\eta)^q(1 + 4\eta)c_3(1 + |t|)^{-d}\end{aligned}$$

The last step follows from the lemma proved after the completion of this proof. Therefore $|||(\mathscr{J}\psi)(t)||| < \infty$. We now define

$$(\mathscr{M}\psi)(t) = e^{-iAt}\varphi_- + (\mathscr{J}\psi)(t)$$

and choose η_0 (and δ in the case $q = 1$) small enough so that

$$\beta(2\eta_0)^{q+1} \int_{-\infty}^{\infty} (1 + |s|)^{-dq}\, ds \le \tfrac{1}{2}\eta_0$$

$$c_2 \beta(2\eta_0)^q (1 + 4\eta_0)c_3 \le \tfrac{1}{2}\eta_0 \tag{258}$$

It is easy to check that $(\mathscr{M}\psi)(t)$ is continuous. Thus, for $\eta \le \eta_0$, $\mathscr{M}$ maps X_{η,φ_-} into itself. Further, it is easy to check using (253) that by choosing η_0 still smaller (and δ in the case $q = 1$) we can guarantee that $\mathscr{M}$ is a contraction. Thus, since X_{η,φ_-} is a complete metric space, $\mathscr{M}$ has a unique fixed point $\varphi(\cdot)$ in X_{η,φ_-}. By the definition of $\mathscr{M}$, $\varphi(\cdot)$ is a global solution of (255). Notice also that $|||\varphi(\cdot)||| \le 2\eta_0$.

To prove uniqueness, let φ_1 be another solution of (255) with $|||\varphi_1(\cdot)||| < \infty$. Then

$$\begin{aligned}
\|\varphi(t) - \varphi_1(t)\| &\le \int_{-\infty}^{t} \|J(\varphi(s)) - J(\varphi_1(s))\|\, ds \\
&\le \int_{-\infty}^{t} \beta(\|\varphi(s)\|_a + \|\varphi_1(s)\|_a)^q \|\varphi(s) - \varphi_1(s)\|\, ds \\
&\le \beta(|||\varphi(\cdot)||| + |||\varphi_1(\cdot)|||)^q \Big(\sup_{-\infty < s \le t} \|\varphi(s) - \varphi_1(s)\|\Big) \\
&\qquad \times \int_{-\infty}^{t} (1 + |s|)^{-dq}\, ds
\end{aligned}$$

so

$$\begin{aligned}
&\sup_{-\infty < s \le t} \|\varphi(s) - \varphi_1(s)\| \\
&\quad \le \left\{\beta(|||\varphi(\cdot)||| + |||\varphi_1(\cdot)|||)^q \int_{-\infty}^{t} (1 + |s|)^{-dq}\, ds\right\} \sup_{-\infty < s \le t} \|\varphi(s) - \varphi_1(s)\|
\end{aligned}$$

But this gives a contradiction for t sufficiently close to $-\infty$ unless $\varphi(s) = \varphi_1(s)$ for all $s \le t$. By local uniqueness (proven by the contraction mapping method as above but starting with initial data given at a finite t), $\varphi(s) = \varphi_1(s)$ for all s.

To show that $\varphi(t) \in \Sigma_{\text{scat}}$ for each t, we fix t and compute:

$$\begin{aligned}
\sup_r \|e^{-irA}\varphi(t)\| &\le \sup_r \|e^{-irA}e^{-itA}\varphi_-\| + \int_{-\infty}^{t} \|e^{-iA(t+r-s)}J(\varphi(s))\|\, ds \\
&\le \sup_r \|e^{-irA}\varphi_-\| + \beta \int_{-\infty}^{t} \|\varphi(s)\|_a^q \|\varphi(s)\|\, ds \\
&\le \|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0
\end{aligned}$$

$$\begin{aligned}
&\sup_r \{(1+|r|)^d \|e^{-irA}\varphi(t)\|_a\} \\
&\qquad \le \sup_r \{(1+|r|)^d \|e^{-i(t+r)A}\varphi_-\|_a\} \\
&\qquad\quad + \sup_r \left\{(1+|r|)^d \int_{-\infty}^{t} \|e^{-iA(t+r-s)}J(\varphi(s))\|_a\, ds\right\} \\
&\qquad \le \sup_r \{(1+|r|)^d(1+|t+r|)^{-d}\|\varphi_-\|_{\text{scat}}\} \\
&\qquad\quad + \sup_r \left\{(1+|r|)^d \int_{-\infty}^{t} (1+|t+r-s|)^{-d}(1+|s|)^{-dq}\, ds\right\} \\
&\qquad\quad \times \beta c_2(1+4\eta_0)(2\eta_0)^q \\
&\qquad \le \sup_r \{(1+|r|)^d(1+|t+r|)^{-d}\}(\|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0)
\end{aligned}$$

Thus, $\varphi(t) \in \Sigma_{\text{scat}}$.

To prove (b), we estimate

$$\begin{aligned}
\|\varphi(t) - e^{-itA}\varphi_-\| &= \|e^{itA}\varphi(t) - \varphi_-\| \\
&\le \int_{-\infty}^{t} \|e^{isA}J(\varphi(s))\|\, ds \\
&\le \beta \int_{-\infty}^{t} \|\varphi(s)\|_a^q \|\varphi(s)\|\, ds \\
&\le \beta(2\eta_0)^{q+1} \int_{-\infty}^{t} (1+|s|)^{-dq}\, ds \\
&\to 0
\end{aligned}$$

as $t \to -\infty$. ▮

The solution of (255) constructed above satisfies (249b) with

$$\varphi_0 = \varphi_- + \int_{-\infty}^{0} e^{iAs} J(\varphi(s))\, ds$$

Part (a) of the following lemma completes the proof of Theorem XI.97. Part (b) is used in the proof of Theorem XI.100.

Lemma 1

(a) Suppose that $q \geq 1$, $d > 0$, and $dq > 1$. Then

$$\int_{-\infty}^{\infty} (1 + |t - s|)^{-d}(1 + |s|)^{-dq}\, ds \leq c_3(1 + |t|)^{-d}$$

(b) Suppose that $q > 1$, $d > 0$, and $dq > 1$. Then

$$\sup_r \left\{(1 + |r|)^d \int_{t_1}^{t_2} (1 + |r - s|)^{-d}(1 + |s|)^{-dq}\, ds\right\} \to 0$$

as $t_1, t_2 \to +\infty$ or $t_1, t_2 \to -\infty$.

Proof (a) It is sufficient to consider the case where t is positive. We break the integral into two parts and estimate:

$$\begin{aligned}\int_{|s-t| \geq t/2} & (1 + |t - s|)^{-d}(1 + |s|)^{-dq}\, ds \\ & \leq \left(1 + \frac{t}{2}\right)^{-d} \int_{|s-t| \geq t/2} (1 + |s|)^{-dq}\, ds \\ & \leq c(1 + t)^{-d} \int_{-\infty}^{\infty} (1 + |s|)^{-dq}\, ds\end{aligned}$$

and for $d \neq 1$,

$$\begin{aligned}\int_{t/2}^{3t/2} & (1 + |t - s|)^{-d}(1 + |s|)^{-dq}\, ds \\ & \leq \left(1 + \frac{t}{2}\right)^{-dq} \left\{\int_{t/2}^{t} (1 + (t - s))^{-d}\, ds + \int_{t}^{3t/2} (1 + s - t)^{-d}\, ds\right\} \\ & \leq 2\left(1 + \frac{t}{2}\right)^{-dq} \left\{|1 - d|^{-1}\left(\left(1 + \frac{t}{2}\right)^{-d+1} + 1\right)\right\} \\ & \leq c(1 + t)^{-dq-d+1} + c(1 + t)^{-dq} \\ & \leq c(1 + t)^{-d}\end{aligned}$$

since $dq > 1$ and $q \geq 1$.

If $d = 1$, the second integral can be estimated by

$$2\left(1+\frac{t}{2}\right)^{-q}\ln\left(1+\frac{t}{2}\right) \le c(1+t)^{-1}$$

since $q > 1$ if $d = 1$.

(b) Consider the case $t_2 > t_1 \to \infty$ and choose $q_0 \ge 1$ so that $dq_0 > 1$ and $q > q_0$. Then

$$(1+|r|^d)\int_{t_1}^{t_2}(1+|r-s|)^{-d}(1+|s|)^{-dq}\,ds$$

$$\le [(1+|t_1|)^{-d(q-q_0)}](1+|r|)^d\int_{-\infty}^{\infty}(1+|r-s|)^{-d}(1+|s|)^{-dq_0}\,ds$$

so (b) follows from (a). ∎

Theorem XI.98 (the scattering operator for small data) Assume all the hypotheses of Theorem XI.97 and let $\varphi(t)$ be the solution of (255) corresponding to $\varphi_- \in \Sigma_{\text{scat}}$ with $\|\varphi_-\|_{\text{scat}} \le \eta_0$. Then, for η_0 sufficiently small:

(a) There exists $\varphi_+ \in \Sigma_{\text{scat}}$, with $\|\varphi_+\|_{\text{scat}} \le 2\eta_0$, so that

$$\|\varphi(t) - e^{-itA}\varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

(b) The map $\varphi_- \xrightarrow{S} \varphi_+$, defined on $\{\varphi \mid \|\varphi_-\|_{\text{scat}} < \eta_0\}$ is one-to-one and continuous in the $\|\cdot\|_{\text{scat}}$ norm.

Proof From Theorem XI.97 we know that $|||\varphi(\cdot)||| \le 2\eta_0$. Thus

$$\|e^{it_1A}\varphi(t_1) - e^{it_2A}\varphi(t_2)\| \le \left\|\int_{t_1}^{t_2} e^{isA}J(\varphi(s))\,ds\right\|$$

$$\le \int_{t_1}^{t_2}\beta\|\varphi(s)\|_a^q\|\varphi(s)\|\,ds$$

$$\le \beta(2\eta_0)^{q+1}\int_{t_1}^{t_2}(1+|s|)^{-dq}\,ds$$

by (252). Thus $\{e^{itA}\varphi(t)\}$ is Cauchy in $\mathscr{H}$ as $t \to +\infty$ since $dq > 1$. Letting

$$\varphi_+ = \lim_{t\to+\infty} e^{itA}\varphi(t)$$

we have

$$\|\varphi(t) - e^{-itA}\varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

by the unitarity of e^{-itA}. To show that $\varphi_+ \in \Sigma_{\text{scat}}$, observe that

$$e^{itA}\varphi(t) = \varphi_- + \int_{-\infty}^{t} e^{isA}J(\varphi(s))\,ds$$

Letting $t \to +\infty$, we conclude that

$$\varphi_+ = \varphi_- + \int_{-\infty}^{\infty} e^{isA}J(\varphi(s))\,ds$$

Now, by (254) and (252),

$$\begin{aligned}\|e^{-iA(t-s)}J(\varphi(s))\|_a &\le c_2(1 + |t-s|)^{-d}\{\|J(\varphi(s))\| + \|J(\varphi(s))\|_b\}\\ &\le c_2\beta(1 + |t-s|)^{-d}\{\|\varphi(s)\|_a^q(1 + 2\|\varphi(s)\|)\}\\ &\le c_2\beta(2\eta_0)^q(1 + 4\eta_0)(1 + |t-s|)^{-d}(1 + |s|)^{-dq}\end{aligned}$$

for each s and t. Since

$$e^{-itA}\varphi_+ = e^{-itA}\varphi_- + \int_{-\infty}^{\infty} e^{-iA(t-s)}J(\varphi(s))\,ds$$

we conclude that $\|e^{-itA}\varphi_+\|_a < \infty$ and

$$\begin{aligned}&\sup_t \{(1 + |t|)^d\|e^{-itA}\varphi_+\|_a\}\\ &\qquad\le \sup_t \{(1 + |t|)^d\|e^{-itA}\varphi_-\|_a\} + c_2\beta(2\eta_0)^q(1 + 4\eta_0)\\ &\qquad\quad\times \sup_t \left\{(1 + |t|)^d\int_{-\infty}^{\infty}(1 + |t-s|)^{-d}(1 + |s|)^{-dq}\,ds\right\}\\ &\qquad\le \sup_t (1 + |t|)^d\|e^{-itA}\varphi_-\|_a + \tfrac{1}{2}\eta_0\end{aligned}$$

by the lemma (part a) and the choice of η_0 in Theorem XI.97. Thus

$$\|\varphi_+\|_{\text{scat}} \le \|\varphi_-\|_{\text{scat}} + \tfrac{1}{2}\eta_0 + \tfrac{1}{2}\eta_0 \le 2\eta_0$$

This proves (a).

To prove that S is continuous, let φ_- and ψ_- be in Σ_{scat} with $\|\varphi_-\|_{\text{scat}} \le \eta_0$ and $\|\psi_-\|_{\text{scat}} \le \eta_0$ and let $\varphi(t)$ and $\psi(t)$ be the corresponding solutions given by Theorem XI.97. We shall first show that $|||\varphi(\cdot) - \psi(\cdot)|||$ can be estimated by $\|\varphi_- - \psi_-\|_{\text{scat}}$ and then show that $\|\varphi_+ - \psi_+\|_{\text{scat}}$ can be estimated by $|||\varphi(\cdot) - \psi(\cdot)|||$. Since

$$\varphi(t) - \psi(t) = e^{-iAt}(\varphi_- - \psi_-) + \int_{-\infty}^{t} e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\,ds$$

we have

$$\begin{aligned}\|\varphi(t)-\psi(t)\| &\le \|\varphi_- - \psi_-\| + \int_{-\infty}^{t} \|J(\varphi(s)) - J(\psi(s))\|\,ds \\ &\le \|\varphi_- - \psi_-\| + \beta(2\eta_0)^q \int_{-\infty}^{t} (1+|s|)^{-dq}\|\varphi(s)-\psi(s)\|\,ds \\ &\le \|\varphi_- - \psi_-\| + \beta(2\eta_0)^q\left(\int_{-\infty}^{\infty}(1+|s|)^{-dq}\,ds\right)|||\varphi(\cdot)-\psi(\cdot)|||\end{aligned}$$

Similarly,

$$\begin{aligned}&\|\varphi(t)-\psi(t)\|_a \\ &\quad\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a + \int_{-\infty}^{t}\|e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\|_a\,ds \\ &\quad\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a \\ &\qquad + c_2\int_{-\infty}^{t}(1+|t-s|)^{-d}\{\|J(\varphi(s)) - J(\psi(s))\|_b + \|J(\varphi(s)) - J(\psi(s))\|\}\,ds \\ &\quad\le \|e^{-iAt}(\varphi_- - \psi_-)\|_a \\ &\qquad + 3c_2\beta(2\eta_0)^q\left(\int_{-\infty}^{\infty}(1+|t-s|)^{-d}(1+|s|)^{-dq}\,ds\right)|||\varphi(\cdot)-\psi(\cdot)|||\end{aligned}$$

Combining these two estimates, we have

$$|||\varphi(\cdot)-\psi(\cdot)||| \le \|\varphi_- - \psi_-\|_{\text{scat}} + c(\beta,\eta_0)|||\varphi(\cdot)-\psi(\cdot)|||$$

where

$$\begin{aligned}c(\beta,\eta_0) &= \beta(2\eta_0)^q\int_{-\infty}^{\infty}(1+|s|)^{-dq}\,ds \\ &\qquad + 3c_2\beta(2\eta_0)^q\sup_t\left\{(1+|t|)^d\int_{-\infty}^{\infty}(1+|t-s|)^{-d}(1+|s|)^{-dq}\,ds\right\}\end{aligned}$$

By choosing η_0 small enough, we can guarantee that $c(\beta,\eta_0)\le\frac{1}{2}$ implying that

$$|||\varphi(\cdot)-\psi(\cdot)||| \le 2\|\varphi_- - \psi_-\|_{\text{scat}} \tag{259}$$

Next

$$\|\varphi_+ - \psi_+\|_{\text{scat}} \leq \|\varphi_- - \psi_-\|_{\text{scat}} + \left\| \int_{-\infty}^{\infty} e^{isA}(J(\varphi(s)) - J(\psi(s)))\, ds \right\|_{\text{scat}}$$

Using the usual estimates, we find that

$$\sup_t \left\| \int_{-\infty}^{\infty} e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\, ds \right\| \leq c(\beta, \eta_0)|||\varphi(\cdot) - \psi(\cdot)|||$$

and

$$\sup_t \left\{ (1 + |t|)^d \left\| \int_{-\infty}^{\infty} e^{-iA(t-s)}(J(\varphi(s)) - J(\psi(s)))\, ds \right\|_a \right\}$$
$$\leq c(\beta, \eta_0)|||\varphi(\cdot) - \psi(\cdot)|||$$

so

$$\begin{aligned} \|\varphi_+ - \psi_+\|_{\text{scat}} &\leq \|\varphi_- - \psi_-\|_{\text{scat}} + c(\beta, \eta_0)|||\varphi(\cdot) - \psi(\cdot)||| \\ &\leq 2\|\varphi_- - \psi_-\|_{\text{scat}} \end{aligned}$$

by (259) above. This proves that S is uniformly $\|\cdot\|_{\text{scat}}$ continuous for η_0 small enough. The proof that S is one-to-one is left to the reader (Problem 126). ▮

Before going on to examples, let us point out several important aspects of these theorems. First, the hypotheses do not require a priori estimates on the solution of the nonlinear equation, nor did we use energy inequalities. The only requirement was that solutions of the *linear* equation decay sufficiently rapidly and that the nonlinearity have high enough degree at zero. In particular, the verification of (i)–(iii) does not depend on the sign of the nonlinear term. Secondly, suppose that the nonlinear equation is of the form

$$\varphi'(t) = -iA\varphi(t) + \lambda J(\varphi(t)) \tag{260}$$

and (i)–(iii) hold. Then for any $\varphi_- \in \Sigma_{\text{scat}}$, the conclusions of Theorems XI.97 and XI.98 hold for λ small enough (the choice of λ depends on $\|\varphi_-\|_{\text{scat}}$). Finally, by slightly rearranging the proofs of the above theorems, we have global existence for the initial value problem at $t = 0$ if the data are small.

Theorem XI.99 Let A, $\mathscr{H}$, and J satisfy the hypotheses of Theorem XI.97. Then for η_0 small enough and any $\varphi_0 \in \Sigma_{\text{scat}}$ with $\|\varphi_0\|_{\text{scat}} \leq \eta_0$, the equation (249b) has a strongly continuous, global, Σ_{scat}-valued solution $\varphi(t)$ so that $\varphi(0) = \varphi_0$. Further, there exist φ_+, φ_- in Σ_{scat} so that

$$\|\varphi(t) - e^{-iAt}\varphi_+\| \to 0, \qquad t \to +\infty$$
$$\|\varphi(t) - e^{-iAt}\varphi_-\| \to 0, \qquad t \to -\infty$$

For any $\varphi_0 \in \Sigma_{\text{scat}}$, the same conclusion holds for the integral equation corresponding to (260) if λ is small enough (depending on $\|\varphi_0\|_{\text{scat}}$).

Example 1 (the nonlinear Schrödinger equation) We begin with an easy example, the nonlinear Schrödinger equation in one dimension,

$$\begin{aligned} iu_t &= -u_{xx} + \lambda |u|^{p-1}u \\ u(x, 0) &= f(x) \end{aligned} \tag{261}$$

because it illustrates nicely the method for choosing the norms described above. The corresponding free equation is

$$\begin{aligned} u_t - iu_{xx} &= 0 \\ u(x, 0) &= f(x) \end{aligned}$$

and $A = -d^2/dx^2$. The solution can be written explicitly as

$$u(x, t) = (4\pi it)^{-1/2} \int e^{i(x-y)^2/4t} f(y)\, dy$$

and thus

$$\|u(x, t)\|_\infty \le |t|^{-1/2} \|f\|_1$$

Therefore, we choose

$$\|u\|_a = \|u\|_\infty, \qquad \|u\|_b = \|u\|_1$$

We have thus satisfied hypothesis (ii) with $d = \frac{1}{2}$. Notice that we cannot choose $L^2(\mathbb{R})$ as our Hilbert space because it is not true that $\|u\|_\infty \le c\|u\|_2$. However, by the proof of Sobolev's lemma (Theorem IX.24):

$$\|u\|_\infty \le c\|Bu\|_2 \tag{262}$$

where as usual $B = \sqrt{-\Delta + m^2}$. Thus, we take

$$\|u\| = \|Bu\|_2$$

so that hypothesis (i) is satisfied. We must check for which p (iii) holds. In the following calculation we replace $|u|^{p-1}u$ by u^p, take p to be an integer, and treat B as though it were d/dx. By using the techniques of Lemmas 3–5 of Section X.13, one can easily handle the actual case. Letting P be a suitable polynomial, we have

$$\begin{aligned}\|J(u_1) - J(u_2)\| &= |\lambda|\, \|B(u_1^p - u_2^p)\|_2 \\ &= |\lambda| p \|(Bu_1)u_1^{p-1} - (Bu_2)u_2^{p-1}\|_2 \\ &\leq |\lambda| p \|(Bu_1)(u_1 - u_2)P(u_1, u_2)\|_2 \\ &\quad + |\lambda| p \|(Bu_1 - Bu_2)u_2^{p-1}\|_2 \\ &\leq C\|Bu_1\|_2\, \|u_1 - u_2\|_\infty\, \|P(u_1, u_2)\|_\infty \\ &\quad + C\|B(u_1 - u_2)\|_2\, \|u_2^{p-1}\|_\infty \\ &\leq C\|Bu_1\|_2\, \|B(u_1 - u_2)\|_2(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \\ &\quad + C\|B(u_1 - u_2)\|_2\, \|u_2\|_\infty^{p-1} \\ &\leq \beta(\|u_1\|_a + \|u_2\|_a)^{p-2}\|u_1 - u_2\|\end{aligned}$$

for $\|u_1\|$ and $\|u_2\|$ small. Thus, the first hypothesis in (iii) holds with $q = p - 2$. Similarly,

$$\begin{aligned}\|J(u_1) - J(u_2)\|_b &= \|u_1^p - u_2^p\|_1 \\ &= \|(u_1 - u_2)Q(u_1, u_2)\|_1 \\ &\leq C\|B(u_1 - u_2)\|_2(\|u_1\|_2 + \|u_2\|_2)(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \\ &\leq \beta\|u_1 - u_2\|(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2}\end{aligned}$$

for $\|u_1\|$ and $\|u_2\|$ small, so the second part of (iii) also holds with $q = p - 2$. Now, since $d = \frac{1}{2}$ and we need $dq > 1$, we must require $q > 2$. Therefore if $p > 4$, Theorems XI.97–XI.99 provide small data global existence and a scattering theory for equation (261).

Example 2 (the nonlinear Klein–Gordon equation, $n = 1$) In order to discuss the equation

$$u_{tt} - u_{xx} + m^2 u = -\lambda u^p \tag{263}$$

we first need a decay estimate for the linear equation

$$\begin{aligned} u_{tt} - u_{xx} + m^2 u &= 0 \\ u(x, 0) &= f \\ u_t(x, 0) &= g \end{aligned} \tag{264}$$

in terms of tractable norms on the initial data. Thus stationary phase methods are not enough, and we shall have to use the explicit formula for the solution of the linear equation in terms of special functions.

Lemma 2 Suppose that f and g are in $\mathscr{S}(\mathbb{R})$ and let $u(x, t)$ be the solution of (264) with initial data $\langle f, g\rangle$. Then

$$\|u(x, t)\|_\infty \leq C|t|^{-1/2}\{\|f\|_1 + \|f'\|_1 + \|f''\|_1 + \|g'\|_1 + \|g\|_1\} \tag{265}$$

Proof For each t, let $u(t)$ denote $u(\cdot, t)$ as an $L^2(\mathbb{R}^3)$-valued function. $u(t)$ is given by

$$u(t) = \cos(Bt)f + \frac{\sin(Bt)}{B} g$$

or

$$[\widehat{u(t)}](k) = \cos(t\sqrt{k^2 + m^2})\hat{f}(k) + \frac{\sin(t\sqrt{k^2 + m^2})}{\sqrt{k^2 + m^2}} \hat{g}(k)$$

Thus $u(t)$ can be written

$$u(t) = \frac{\partial R}{\partial t} * f + R * g$$

where for each t, R is the inverse Fourier transform

$$R(x, t) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{ikx} \frac{\sin t\sqrt{k^2 + m^2}}{\sqrt{k^2 + m^2}}\, dk$$

in the sense of distributions. The convolution $R * g$ makes sense since $R \in \mathscr{S}'(\mathbb{R})$ and $g \in \mathscr{S}(\mathbb{R})$. There are many ways to figure out what the function $R(x, t)$ is. Here is one. First we notice that $R(x, t)$ is zero except when $x^2 \leq t^2$. This follows from the Paley–Wiener theorem for distributions and the analyticity and growth of $(k^2 + m^2)^{-1/2} \sin t\sqrt{k^2 + m^2}$ in the imaginary k directions. Secondly, we can compute directly that $R(x, t)$ is invariant under two-dimensional Lorentz transformations. Thus for $t > 0$, $R(x, t)$ is a function of $t^2 - x^2$. Suppose that we write for $x^2 \leq t^2$, $t > 0$,

$$H(\sqrt{t^2 - x^2}) \equiv R(x, t) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{ikx} \frac{\sin t\sqrt{k^2 + m^2}}{\sqrt{k^2 + m^2}}\, dk$$

Then, differentiating twice with respect to t and twice with respect to x and subtracting the results, one finds that H satisfies

$$H''(y) + \frac{1}{y} H'(y) + m^2 H(y) = 0$$

so

$$H(y) = cJ_0(my) + dY_0(my)$$

where J_0 and Y_0 are Bessel functions. d must be zero since $R(\cdot, t) \in L^2(\mathbb{R})$ and Y_0 has a $1/y$ singularity at $y = 0$. Setting $x = 0$, one determines that $c = \frac{1}{2}$. Thus, for $t > 0$,

$$R(x, t) = \tfrac{1}{2}\chi_{\{x \mid x^2 \le t^2\}}(x)J_0(m\sqrt{t^2 - x^2})$$

Therefore we have the representation

$$(R * g)(x, t) = \tfrac{1}{2}\int_{-t}^{t} J_0(m\sqrt{t^2 - y^2})g(x - y)\, dy \tag{266}$$

To analyze the decay of $R * g$ we need the estimates

$$J_0(\mu) = \left(\frac{2}{\mu\pi}\right)^{\frac{1}{2}} \cos\left(\mu - \frac{\pi}{4}\right) + O(\mu^{-\frac{3}{2}})$$

$$J_1(\mu) = O(\mu^{-\frac{1}{2}})$$

as $\mu \to \infty$. We write (266) as an integral over $\{y \mid |y| \le \frac{1}{2}t\}$ and an integral over $\{y \mid \frac{1}{2}t \le |y| \le t\}$. Using $|J_0(\mu)| \le c\mu^{-1/2}$, the first can easily be estimated by

$$ct^{-1/2}\int_{-\frac{1}{2}t}^{\frac{1}{2}t} |g(x - y)|\, dy \le ct^{-1/2}\|g\|_1 \tag{267}$$

There are two integrals left, one of which is

$$\begin{aligned}
&\tfrac{1}{2}\int_{\frac{1}{2}t}^{t} J_0(m\sqrt{t^2 - y^2})g(x - y)\, dy \\
&\quad = \left(\frac{1}{2\pi m}\right)^{1/2} \int_{\frac{1}{2}t}^{t} \frac{\cos(m\sqrt{t^2 - y^2} - \frac{1}{4}\pi)}{(t^2 - y^2)^{1/4}} g(x - y)\, dy \\
&\quad\quad + \int_{\frac{1}{2}t}^{t} O((t^2 - y^2)^{-3/4})g(x - y)\, dy
\end{aligned}$$

For the second term, we have

$$\begin{aligned}
\int_{\frac{1}{2}t}^{t} O((t^2 - y^2)^{-3/4})g(x - y)\, dy &\le ct^{-3/4}\|g\|_\infty \int_{\frac{1}{2}t}^{t} (t - y)^{-3/4}\, dy \\
&\le ct^{-1/2}\|g\|_\infty
\end{aligned}$$

To handle the first term, we integrate by parts obtaining:

$$-g(x-y)\frac{(t^2-y^2)^{1/4}}{my\sqrt{2\pi m}}\sin\left(m\sqrt{t^2-y^2}-\frac{\pi}{4}\right)\Bigg]_{y=\frac{1}{2}t}^{y=t}$$
$$+\frac{1}{m\sqrt{2\pi m}}\int_{\frac{1}{2}t}^{t}\sin\left(m\sqrt{t^2-y^2}-\frac{\pi}{4}\right)\frac{d}{dy}\left\{\frac{(t^2-y^2)^{1/4}}{y}g(x-y)\right\}dy$$

Both terms may be easily estimated by $ct^{-1/2}(\|g\|_1+\|g'\|_1)$. Combining this with (267), we have

$$\|R*g\|_\infty\le ct^{-1/2}(\|g\|_1+\|g'\|_1)$$

To treat the $(\partial R/\partial t)*f$ term, notice that

$$\frac{\partial R}{\partial t}=\frac{1}{2}(\delta(x+t)+\delta(x-t))+\frac{1}{2}m\frac{t}{\sqrt{t^2-x^2}}J_1(m\sqrt{t^2-x^2})$$

so

$$\left(\frac{\partial R}{\partial t}*f\right)(x,t)=\frac{1}{2}\{f(x+t)+f(x-t)\}$$
$$+\frac{1}{2}m\int_{-t}^{t}\frac{t}{\sqrt{t^2-y^2}}J_1(m\sqrt{t^2-y^2})f(x-y)\,dy \tag{268}$$

First we estimate the integral over $\{y\,|\,|y|\le\frac{1}{2}t\}$ as before. Then we integrate the remaining integral by parts, observe that the boundary terms at $y=\pm t$ cancel the first term in (268), and estimate the other boundary terms and the remaining integral by a second integration by parts just as we did for $R*g$. The result is

$$\left\|\left(\frac{\partial R}{\partial t}*f\right)\right\|_\infty\le ct^{-1/2}(\|f\|_1+\|f'\|_1+\|f''\|_1)$$

The extra derivative on f occurs because there was one extra integration by parts. This proves the lemma. ∎

For f and g nice, this lemma gives us a decay estimate and leads us to define

$$\|\langle u,v\rangle\|_a=\|u\|_\infty$$
$$\|\langle u,v\rangle\|_b=\|u\|_1+\|u'\|_1+\|u''\|_1+\|v\|_1+\|v'\|_1$$

We take as our Hilbert space

$$\mathscr{H}=\left\{\varphi=\langle u,v\rangle\,\middle|\,\|\varphi\|^2=\|Bu\|_2^2+\|v\|_2^2<\infty\right\}$$

Then, by (262), (i) holds. By the lemma,

$$\|e^{-itA}\varphi\|_a \leq c|t|^{-1/2}\|\varphi\|_b$$

for nice φ. By the linearity, this extends to all $\varphi \in \mathscr{H}$. Thus we have (ii). It remains to check for which p (iii) holds. Since $J(\varphi) = \langle 0, -\lambda u^p\rangle$,

$$\begin{aligned}
\|J(\varphi_1) - J(\varphi_2)\| &\leq |\lambda| \, \|u_1^p - u_2^p\|_2 \\
&\leq c|\lambda| \, \|u_1 - u_2\|_2(\|u_1\|_\infty + \|u_2\|_\infty)^{p-1} \\
&\leq c|\lambda|(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-1}\|\varphi_1 - \varphi_2\| \\
\|J(\varphi_1) - J(\varphi_2)\|_b &= |\lambda|\{\|u_1^p - u_2^p\|_1 + \|(u_1^p - u_2^p)'\|_1\} \\
&\leq c|\lambda|\{\|u_1 - u_2\|_2 + \|u_1' - u_2'\|_2\} \\
&\quad \times (\|u_1\|_2 + \|u_2\|_2)(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2} \\
&\leq |\lambda|(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-2}\|\varphi_1 - \varphi_2\|
\end{aligned}$$

Thus, the estimates in hypothesis (iii) are satisfied with $q = p - 2$. Since $d = \frac{1}{2}$ and we need $dq > 1$, we must choose $q > 2$ so $p > 4$. We have thus proven, by Theorems XI.97–XI.99, global existence for small Cauchy data and the existence of the scattering operator for small data if $p > 4$. Notice that this result holds whatever the sign of λ and whether p is either even or odd (or fractional).

Example 3 (nonlinear Klein–Gordon equation, $n = 3$) In order to handle the nonlinear Klein–Gordon equation (245) with $F(u) = -\lambda|u|^{p-1}u$ in three dimensions we first need a lemma which is analogous to Lemma 2.

Lemma 3 Let $f, g \in \mathscr{S}(\mathbb{R}^3)$ and let $u(x, t)$ be the solution of

$$u_{tt} - \Delta u + m^2 u = 0$$

$$u(x, 0) = f(x)$$

$$u_t(x, 0) = g(x)$$

Then, there is a universal constant c so that

$$\|u(x, t)\|_\infty \leq c|t|^{-3/2}\|\langle f, g\rangle\|_b \tag{269}$$

where $\|\langle f, g\rangle\|_b$ is defined as the sum of the L_1 norms of all the derivatives of f of order ≤ 3 and all the derivatives of g of order ≤ 2.

The proof of this lemma is similar to the proof of Lemma 2; only the determination of the form of $R(x, t)$ is a little more complicated. The extra derivative on the initial data comes about because $R(x, t)$ itself involves J_1. Thus, one must integrate by parts twice for the g terms and three times for the f terms. We spare the reader the details.

So, we choose $\|\varphi\|_b$ to be as defined in the lemma and $\|\varphi\|_a = \|u\|_\infty$. Then, (ii) is satisfied with $d = \frac{3}{2}$. However, we can no longer use the Hilbert space $\mathscr{H}$ because it is not true that $\|u\|_\infty \le c\|Bu\|_2$ in three dimensions. It *is* true that $\|u\|_\infty \le c\|B^2u\|_2$, so we can use

$$\|\langle u, v\rangle\|^2 = \|B^2u\|_2^2 + \|Bv\|_2^2$$

$$\mathscr{H}_1 = \left\{\langle u, v\rangle \,\middle|\, \|\langle u, v\rangle\| < \infty\right\}$$

Then, the free dynamics is unitary on $\mathscr{H}_1$ and (i) holds. Further, similar calculations to those in one dimension show that

$$\begin{aligned}\|J(\varphi_1) - J(\varphi_2)\| &= |\lambda|\, \|B(u_1^p - u_2^p)\|_2 \\ &\le |\lambda|(\|\varphi_1\| + \|\varphi_2\|)(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-2}\|\varphi_1 - \varphi_2\|\end{aligned}$$

There are many terms in $\|J(\varphi_1) - J(\varphi_2)\|_b$. Let us look at one of highest order in D (denote by D_i any partial derivative):

$$\begin{aligned}&\|D_i^2(u_1^p - u_2^p)\|_1 \\ &\quad\le \|(D_i^2(u_1 - u_2))P(u_1, u_2)\|_1 + 2\|(D_i(u_1 - u_2))D_i P(u_1, u_2)\|_1 \\ &\qquad + \|(u_1 - u_2)D_i^2 P(u_1, u_2)\|_1 \\ &\quad\le C(\|Bu_1\|_2 + \|Bu_2\|_2)(\|u_1\|_\infty + \|u_2\|_\infty)^{p-2}\|B^2(u_1 - u_2)\|_2 \\ &\qquad + C(\|Bu_1\|_2 + \|Bu_2\|_2)^2(\|u_1\|_\infty + \|u_2\|_\infty)^{p-3}\|u_1 - u_2\|_\infty \\ &\quad\le \beta\{(\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-3}\|\varphi_1 - \varphi_2\|_a + (\|\varphi_1\|_a + \|\varphi_2\|_a)^{p-2}\|\varphi_1 - \varphi_2\|\}\end{aligned}$$

Thus, (iii) is satisfied with $q = p - 2$ for slightly different reasons than in one dimension (you should not assume that $q = p - 2$ is all right in all dimensions). Notice in the case $q = 1$, the constant β in (iii) is small if $\|\varphi_1\| + \|\varphi_2\|$ is small. Since $d = \frac{3}{2}$, we need only choose $q \ge 1$, so $p \ge 3$. For all such p, we have a scattering theory and global existence for the equation

$$u_{tt} - \Delta u + m^2u = -\lambda|u|^{p-1}u, \qquad x \in \mathbb{R}^3 \tag{270}$$

for small data independent of whether p is even or odd and of the sign of λ.

In order to discuss scattering for solutions of nonlinear equations where neither the data nor the coupling constant is small one needs global existence results. Thus, unlike the case of small data, the nonlinear terms usually have to have the right signs so that there is a conserved energy that is bounded below. Using such a conserved quantity, one shows that the norm of any local solution cannot go to infinity in finite time and thus that global solutions exist (see Section X.13). If we have global existence, then we can construct the wave operators by methods similar to those that we used in the case of small data. In the following we denote by M_t the group of *nonlinear* operators

$$M_t\colon \varphi_0 \to \varphi(t)$$

where $\varphi(t)$ solves

$$\varphi(t) = e^{-itA}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds \tag{249b}$$

Theorem XI.100 (existence of the wave operators) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a nonlinear mapping of $\mathscr{H}$ into itself. Suppose that there exist norms $\|\cdot\|_a$, $\|\cdot\|_b$ so that the hypotheses (i)–(iii) hold with $q > 1$. Suppose that for each η and T, the solutions $M_t\varphi_0$ of (249b) are uniformly bounded (in $\|\cdot\|$-norm) for all $\|\varphi_0\| \le \eta$ and all $0 < |t| \le T$. Then:

(a) For each $\varphi_- \in \Sigma_{\text{scat}}$, there is a unique global solution $\varphi(\cdot)$ of (249b) so that $\varphi(t) \in \Sigma_{\text{scat}}$ for each t, and

$$\|\varphi(t) - e^{-iAt}\varphi_-\| \to 0 \qquad \text{as} \quad t \to -\infty$$

(b) The mapping $\Omega^+ : \varphi_- \to \varphi(0)$ is a one-to-one map of Σ_{scat} into Σ_{scat} that is uniformly continuous on balls in Σ_{scat}.

(c) Analogous statements as in (a) and (b) hold for $\varphi_+ \in \Sigma_{\text{scat}}$, $t \to +\infty$, and the map $\Omega^- : \varphi_+ \to \varphi(0)$.

Proof We just sketch the proof since the details are very similar to the case of small data. Let $\varphi_- \in \Sigma_{\text{scat}}$ be given, $\|\varphi_-\|_{\text{scat}} \le \eta$ (note that η is not assumed small). Let $X_{\eta,\varphi_-,T}$ denote the $\mathscr{H}$-valued continuous functions $\psi(\cdot)$ on $(-\infty, T]$ so that

$$\begin{aligned} &|||\psi(t) - e^{-itA}\varphi_-|||_{(-\infty,T]} \\ &\quad \equiv \sup_{-\infty \le t \le T} \|\psi(t) - e^{-itA}\varphi_-\| + \sup_{-\infty \le t \le T} (1 + |t|)^d \|\psi(t) - e^{-itA}\varphi_-\|_a \\ &\quad \le \eta \end{aligned}$$

For each T, $X_{\eta,\varphi_-,T}$ is a complete metric space. We define $\mathscr{J}$ and $\mathscr{M}$ as before so that

$$(\mathscr{M}\psi)(t) = e^{-iAt}\varphi_- + (\mathscr{J}\psi)(t)$$

The estimates (256) and (257) of Theorem XI.97 show that $|||(\mathscr{J}\psi)(t)|||_{(-\infty,T)}$ is small and that $\mathscr{M}$ is a contraction so long as T is sufficiently close to $-\infty$. (Since the data are not small, the smallness must come from part (b) of Lemma 1, which is why we require $q > 1$.) Thus $\mathscr{M}$ has a fixed point in X_{η,φ_-,T_0} for some fixed T_0. Just as in Theorem XI.97, one can prove that $\varphi(t) \in \Sigma_{\text{scat}}$ for each $t \in (-\infty, T_0]$ and that the limits in (a) hold.

By the estimates (256) and (257), we can use the same T_0 for all φ_- with $\|\varphi_-\| \le \eta$. Thus, we can define the map

$$\Omega^+_{T_0}\colon \varphi_- \mapsto \varphi(T_0)$$

on $\mathscr{B}_\eta \equiv \{\psi \in \Sigma_{\text{scat}} \mid \|\psi\|_{\text{scat}} \le \eta\}$ and as in Theorems XI.97 and XI.98, $\Omega^+_{T_0}$ is a one-to-one uniformly continuous map of $\mathscr{B}_\eta$ into Σ_{scat}. Thus far, global existence has not been used.

It can easily be checked that for $t \le T_0$ our solution $\varphi(t)$ satisfies

$$\varphi(t) = e^{-iA(t-T_0)}\varphi(T_0) + \int_{T_0}^{t} e^{-iA(t-s)}J(\varphi(s))\,ds$$

Since J is Lipschitz, this equation can be solved locally in a neighborhood of T_0 by $\varphi(t) = M_{t-T_0}\varphi(T_0)$; by the boundedness hypothesis on M_t, this solution is global in t. By local uniqueness this definition of $\varphi(t)$ coincides with the $\varphi(t)$ defined earlier for $t \le T_0$. It is easy to check that $\varphi(t)$ satisfies (249b) and that (254) and (253) imply that $\varphi(t)$ is in Σ_{scat} for all t. In fact, the uniform boundedness of M_t assumed in the hypotheses combined with (253) and (254) imply that for each t and each η_0, M_t is a uniformly continuous one-to-one map of $\mathscr{B}_{\eta_0}$ into Σ_{scat} (Problem 128). Thus, for each η, we define

$$\Omega^+ = M_{-T_0}\Omega^+_{T_0}$$

that is,

$$\Omega^+\colon \varphi_- \to \varphi(0)$$

We note that T_0 depends on η. By the properties of M_{-T_0} and $\Omega^+_{T_0(\eta)}$, we have that Ω^+ is a one-to-one uniformly continuous map of $\mathscr{B}_\eta$ into Σ_{scat}. Since η was arbitrary, Ω^+ takes Σ_{scat} into Σ_{scat} and is uniformly continuous on balls. An easy argument shows that Ω^+ is one-to-one on all of Σ_{scat}. This proves (a) and (b); the proof of (c) is similar. ∎

Examples 1 and 2, revisited To prove existence of the wave operators we need just check global existence and uniform continuity. For the nonlinear Klein–Gordon equation, this was done for $\lambda > 0$, $p \geq 1$ in Problem 75 of Chapter X. Similar methods (Problem 130) work for the nonlinear Schrödinger equations, using the Hilbert space of Example 1 and the conserved quantities

$$\int_{\mathbb{R}} |u(x, t)|^2 \, dx, \qquad \int_{\mathbb{R}} \frac{1}{2} |u_x(x, t)|^2 + \frac{1}{p+1} |u(x, t)|^{p+1} \, dx$$

Thus, by Theorem XI.100 and the analysis of Examples 1 and 2, the wave operators exist if $p > 4$ and $\lambda > 0$.

Example 3, revisited For the case $n = 3$, we computed in Example 3 that the hypotheses (i)–(iii) hold with $d = \frac{3}{2}$ and $q = p - 2$. Since we must have $q > 1$ in Theorem XI.100, we must take $p > 3$. For $p \geq 5$, the global existence of strong solutions to (270) is open; For $p = 3$, the methods of Section X.13 give global existence and uniform continuity on balls. For the borderline case $p = 3$, one can get around the fact that Theorem XI.100 does not hold when $q = 1$ by using the following special estimates:

$$\begin{aligned} \|e^{-iA(t-s)} J(\varphi(s))\|_a &= \|B^{-1} \sin[(t-s)B] u^3(s)\|_\infty \\ &\leq C \|B u^3(s)\|_2 \\ &\leq C \|\varphi(s)\| \, \|\varphi(s)\|_a^2 \end{aligned}$$

With this estimate the proof of Theorem XI.100 goes through in the case $p = 3$. The reader is asked to provide the details in Problem 129.

This illustrates a very important point. Since the hypotheses of Theorems XI.97–XI.101 and techniques of proof are quite general, one can often do better in specific applications by using special properties of the particular operators at hand.

As in the quantum-mechanical case, we have now arrived at a really hard problem, the question of asymptotic completeness. To see what is involved let φ_0 be in the range of the Ω^+ constructed in Theorem XI.100. What we must show is that there is a φ_+ so that the solution $\varphi(t)$ of

$$\varphi(t) = e^{-itA} \varphi_0 + \int_0^t e^{-iA(t-s)} J(\varphi(s)) \, ds$$

satisfies

$$\|\varphi(t) - e^{-itA} \varphi_+\| \to 0 \qquad \text{as} \quad t \to +\infty$$

By Cook's method, we should try to construct φ_+ by showing that $e^{itA}\varphi(t)$ is Cauchy in t as $t \to \infty$. Using (249b),

$$\|e^{it_1A}\varphi(t_1) - e^{it_2A}\varphi(t_2)\| \le \int_{t_2}^{t_1} \|J(\varphi(s))\|\, ds$$

So, what we need is

$$\int_{-\infty}^{\infty} \|J(\varphi(s))\|\, ds < \infty \tag{270a}$$

Typically, in order to prove (270a) one needs to prove a priori estimates which guarantee that all solutions of (249) with nice initial data decay sufficiently rapidly in t in appropriate norms. Furthermore, to prove continuity of the scattering operator, the constants in this decay must be estimated in terms of the decay of the corresponding solution of the free equation. As we explained at the beginning of this section, such decay will not hold for general nonlinear equations because of the possibility of bound states. But even when the equation has no bound states, proving an a priori estimate is very difficult. Indeed, only very special cases have been treated. We will indicate the techniques involved by proving:

Theorem XI.101 Let f and g be real-valued functions in $C_0^\infty(\mathbb{R}^3)$ and let u denote the solution of

$$u_{tt} - \Delta u = -u^3, \qquad x \in \mathbb{R}^3, \quad t \in \mathbb{R} \tag{270b}$$

$$u(x, 0) = f(x), \qquad u_t(x, 0) = g(x)$$

Let $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$ and let $\|\varphi\|$ denote the free energy norm, $\|\varphi\|^2 = \|\nabla u\|_2^2 + \|u_t\|_2^2$. Let e^{-itA}, where $A = i\left[\begin{smallmatrix} 0 & I \\ \Delta & 0 \end{smallmatrix}\right]$, be the group corresponding to solutions of the free wave equation $v_{tt} - \Delta v = 0$. Then there exist $\psi_\pm$, satisfying $\|\psi_\pm\| < \infty$, such that $\|\varphi(t) - e^{-itA}\psi_\pm\| \to 0$, as $t \to \pm\infty$.

The existence of smooth solutions of (270b) is discussed in Problem 76 of Chapter X. Using the methods of Section X.13 one can prove that if the initial data are in $C_0^\infty \times C_0^\infty$, then $u(x, t)$ will be in $C_0^\infty \times C_0^\infty$ for all t. Results similar to those in Theorem XI.101 hold for complex-valued solutions if $-u^3$ is replaced by $-u|u|^2$. Theorem XI.101 is not completely satisfactory. Although it does show that solutions of (270b) with nice initial data are asymptotically free, it does not say which $\psi_\pm$ do occur. Thus, we do not have an explicit domain for the scattering operator. Nevertheless, the proof of Theorem XI.101 will illustrate the difficulties that need to be overcome in proving asymptotic completeness results.

Our proof of Theorem XI.101 will rely on the existence of a special conserved quantity, the **conformal charge**,

$$Q_C = \int k_0(\mathbf{x}, t)\, d^3x \tag{270c}$$

where

$$k_0(x, t) = (t^2 + |\mathbf{x}|^2)[\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4] + 2tu_t\, \mathbf{x} \cdot \nabla u + 2tu_t u - u^2 \tag{270d}$$

Using the fact that u satisfies (270b) and has compact support for each t, one can check that Q_C is independent of t. The answer to the more subtle question, How does one find such conserved quantities?, is described in the appendix. In addition, the procedure explains which terms have to be integrated by parts to verify the independence.

Proof of Theorem XI.101 Since $J\langle u, v\rangle = \langle 0, -u^3\rangle$, we have that $\|J(\varphi(s))\| = \|u^3\|_2$. Using the fact that the energy

$$E(t) = \int [\tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{2}u_t^2 + \tfrac{1}{4}u^4]\, d^3x$$

is conserved and the Sobolev estimate $\|u\|_6 \le C\|\sqrt{-\Delta + 1}\, u\|_2$, it follows easily (see Problem 76 in Chapter X) that $\|u(s)^3\|_2$ is bounded as s runs through any compact set. Thus in order to prove that (270a) holds, we must just show that $\|u(s)^3\|_2$ decays sufficiently rapidly at ∞. Writing $\|u(s)^3\|_2 \le \|u(s)\|_\infty \|u(s)^2\|_2$, we shall first use the fact that Q_C is conserved to show that $\|u(s)^2\|_2 \le C|s|^{-1}$ and then use, in addition, a Sobolev estimate and iteration to show that $\|u(s)\|_\infty \le C|s|^{-1/6}$.

We begin by noting that

$$r^{-1}\nabla(ru) = \nabla u + r^{-2}\mathbf{r}u$$

so that

$$(r^2 + t^2)(\nabla u)^2 = (r^2 + t^2)[r^{-1}\nabla(ru)]^2 + r^{-2}(r^2 + t^2)u^2 + A$$

where

$$A = -2u\frac{\partial(ru)}{\partial r} - 2r^{-2}t^2u\frac{\partial(ru)}{\partial r}$$

After some manipulation, one finds that

$$r^2 A = r^2u^2 - t^2u^2 - \frac{\partial}{\partial r}(r^3u^2 + t^2ru^2)$$

so

$$\int_{\mathbb{R}^3} A\, d^3x = \int_{\mathbb{R}^3} u^2 r^{-2}(r^2 - t^2)\, d^3x$$

since $\int r^{-2}(\partial f/\partial r)\, d^3x = -4\pi f(0)$ if f has compact support, is smooth away from zero, and C^1 up to zero. We conclude that

$$\int (r^2 + t^2)(\nabla u)^2\, d^3x = \int [(r^2 + t^2)(r^{-1}\nabla(ru))^2 + 2u^2]\, d^3x$$

so

$$Q_{\mathrm{C}} = \int (t^2 + |x|)^2(\tfrac{1}{4}u^4)\, d^3x + \int B\, d^3x$$

where

$$B = \tfrac{1}{2}(r^2 + t^2)[(r^{-1}\nabla(ru))^2 + u_t^2] + 2tu_t \mathbf{x} \cdot (r^{-1}\nabla(ru))$$

Using $abcd \le [\frac{1}{2}(a^2 + c^2)][\frac{1}{2}(b^2 + d^2)]$, we see that B is positive, so $\int u^4\, d^3x \le 4Q_{\mathrm{C}} t^{-2}$, which yields

$$\|u(t)^2\|_2 \le C|t|^{-1} \tag{270e}$$

Let $\varphi_0 = \langle f, g\rangle$. The first component of $e^{-itA}\langle f, g\rangle$ satisfies the free wave equation and, by (216a), may be represented by

$$[e^{-itA}\langle f, g\rangle]_1 = (4\pi t)^{-1} \int g(x + y)\, dS_{|t|} + \frac{d}{dt}\left[(4\pi t)^{-1} \int f(x + y)\, dS_{|t|}\right]$$

where $dS_{|t|}$ is the usual measure on the sphere of radius $|t|$ (with center at 0), normalized so that $\int dS_{|t|} = 4\pi t^2$. From this explicit representation it immediately follows that, for $f, g \in C_0^\infty(\mathbb{R}^3)$,

$$\|[e^{-itA}\varphi_0]_1\|_\infty \le C(1 + |t|)^{-1} \tag{270f}$$

Moreover,

$$\|[e^{-itA}\langle 0, g\rangle]_1\|_\infty \le C|t|^{-1/2}\|\nabla g\|_{6/5} \tag{270g}$$

To prove this we let $|y| = 1$, $t > 0$, and write

$$|g(y)| \le \int_1^\infty |(\nabla g)(ry)|\, dr$$

so, by Hölder's inequality,

$$\begin{aligned}\left|\int g(y)\,dS_1\right| &\le \int_{S_1}\int_1^\infty (|\nabla g|\,r^{5/3})r^{-5/3}\,dr\,dS_1\\ &\le C\left\{\int_{S_1}\int_1^\infty |\nabla g|^{6/5}r^2\,dr\,dS_1\right\}^{5/6}\end{aligned}$$

where $C = (4\pi\int_1^\infty r^{-10}\,dr)^{1/6} < \infty$. This estimate and scaling imply (for $t > 0$):

$$\left|\frac{1}{4\pi t}\int_{S_t} g(x+y)\,dS_t\right| \le Ct^{-1/2}\left\{\int_{S_1}\int_t^\infty |\nabla g|^{6/5}r^2\,dr\,dS_1\right\}^{5/6}$$

which yields (270g).

Now, suppose that u solves (270b). Then (270f) and (270g) imply (for $t > 0$):

$$\begin{aligned}\|u(\cdot, t)\|_\infty &\le \|[e^{-itA}\varphi_0]_1\|_\infty + \int_0^t \|[e^{-i(t-s)A}\langle 0, -u(s)^3\rangle]_1\|_\infty\,ds\\ &\le C(1+t)^{-1} + C\int_0^t (t-s)^{-1/2}\|\nabla(u(s)^3)\|_{6/5}\,ds\end{aligned}$$

Using (270e) and the fact that $\|\nabla u\|_2$ is a priori bounded by the conservation of energy,

$$\begin{aligned}\|\nabla u^3\|_{6/5} \le 3\|(\nabla u)u^2\|_{6/5} &\le 3\|\nabla u\|_2\,\|u^2\|_3\\ &\le C\|u\|_4^{4/3}\|u\|_\infty^{2/3}\\ &\le C(1+s)^{-2/3}\|u\|_\infty^{2/3}\end{aligned}$$

Thus, if we let $M(t) \equiv \sup_{0\le s\le t}\|u(\cdot, s)\|_\infty$, we have

$$\|u(\cdot, t)\|_\infty \le C(1+t)^{-1} + DM(t)^{2/3}t^{-1/6}$$

where $D = C\int_0^1 (1-\sigma)^{-1/2}\sigma^{-2/3}\,d\sigma < \infty$. From this we first conclude that $\sup_{0\le t<\infty} M(t) < \infty$ and then that

$$\|u(\cdot, t)\|_\infty \le C|t|^{-1/6} \tag{270h}$$

for $t > 0$. The proof for $t < 0$ is similar. (270h) and (270e) imply (270a) and, as indicated above, (270a) implies the result of the theorem. ∎

Appendix to Section XI.13: Conserved currents

One way to see that Q_C, given by (270c), is conserved is to observe that if we define

$$\mathbf{k} = -(\nabla u)\{(|\mathbf{x}|^2 + t^2)u_t + 2t\mathbf{x}\cdot\nabla u + 2tu\} - 2t\mathbf{x}(\tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4) \tag{270i}$$

and use the differential equation (270b), then we can compute that

$$\frac{\partial k_0}{\partial t} + \nabla\cdot\mathbf{k} = 0$$

Thus,

$$\frac{d}{dt}Q_C = \int \frac{\partial k_0}{\partial t}\,d^3x = -\int \nabla\cdot\mathbf{k}\,d^3x = 0$$

where we have used the fact that u, and therefore $\mathbf{k}$, is C^∞ with compact support in x for each t (this follows from the fact that the initial data are in $C_0^\infty(\mathbb{R}^3)$).

The group of ideas, generally called Noether's theorem, which explains how to find such k_0 and $\mathbf{k}$ are the subject of this appendix. They are best described by a Lagrangian formalism which we introduce first. Let $\mathbf{x}$ be in $\mathbb{R}^n$ and u a real-valued function of $\mathbf{x}$ (for the extension to multicomponent u, see Problem 152). Let $\mathscr{L}$ be a function of $n + 2$ real variables $\mathscr{L}(a, \mathbf{b}, c)$, where $a \in \mathbb{R}$, $\mathbf{b} \in \mathbb{R}^n$, $c \in \mathbb{R}$. Given a real-valued function $u(\mathbf{x}, t)$ on $\mathbb{R}^n \times \mathbb{R}$, we form the function $F_u(\mathbf{x}, t) = \mathscr{L}(u_t, \nabla u, u)$ which is a function of $\mathbf{x}$ and t. We shall follow common practice and abuse notation in several ways. First, we shall not call the variables a, $\mathbf{b}$, c, but rather u_t, ∇u, and u. Thus, $\partial\mathscr{L}/\partial u_t$ just means the derivative of $\mathscr{L}$ on $\mathbb{R}^{n+2}$ with respect to its first variable. Moreover, when u is implicitly given, we shall write $\mathscr{L}(x, t)$ or $\mathscr{L}$ for the function denoted by $F_u(x, t)$ above. Thus, for example, a symbol like $(\partial/\partial t)(\partial\mathscr{L}/\partial u_t)$ indicates that we evaluate the function $\partial\mathscr{L}/\partial a$ by using u_t for a, etc., and then take the partial derivative with respect to t of the resulting function of $\mathbf{x}$ and t. And $\partial\mathscr{L}/\partial(\nabla u)$ denotes the n vector $\langle\partial\mathscr{L}/\partial b_1, \ldots, \partial\mathscr{L}/\partial b_n\rangle$ evaluated at u_t, ∇u, u. While these abuses are confusing, they are completely standard in the literature and quite convenient once one gets used to them.

We want to choose $\mathscr{L}$ so that the differential equation under consideration has the form of an **Euler–Lagrange** equation

$$(\mathscr{D})(u) = \frac{\partial}{\partial t}\left(\frac{\partial\mathscr{L}}{\partial u_t}\right) + \nabla\cdot\frac{\partial\mathscr{L}}{\partial(\nabla u)} - \frac{\partial\mathscr{L}}{\partial u} = 0 \tag{270j}$$

(270b) has this form if we choose

$$\mathscr{L}(u_t, \nabla u, u) = \tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4 \tag{270k}$$

The reason that (270j) is so useful involves the **principle of least action** or, more properly, the **principle of stationary action**: Given a bounded open region Ω in $\mathbb{R}^{n+1}$ with smooth boundary and a C^∞ function u on a neighborhood of Ω, we define the **action** by

$$A_\Omega(u) = \int_\Omega \mathscr{L}(u_t, \nabla u, u)\, d^n x\, dt$$

If v is in $C_0^\infty(\Omega)$, that is, v is C^∞ but vanishes near the boundary of Ω, then

$$\frac{d}{d\lambda} A_\Omega(u + \lambda v)\bigg|_{\lambda=0} = -\int_\Omega v(\mathscr{D})(u)\, d^3x\, dt \tag{270l}$$

so u solves (270j) if and only if, for each Ω, the action A_Ω is stationary under small changes of u *strictly inside* Ω. This gives us a way to connect the invariance properties of the equation (270j) with those of $\mathscr{L}$ itself. Consider a smooth change of coordinates

$$s = s(\mathbf{x}, t), \qquad \mathbf{y} = \mathbf{y}(\mathbf{x}, t)$$

and a smooth function V from $\mathbb{R}^{n+2}$ to $\mathbb{R}$. Let $\tilde{u}(\mathbf{x}, t)$ be defined by

$$\tilde{u}(\mathbf{x}, t) = V(u(\mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t)), \mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t))$$

When is it true that $\tilde{u}$ solves (270j) if u does? A *sufficient* condition is that $\delta\mathscr{L} = 0$ where

$$\delta\mathscr{L} \equiv [\mathscr{L}(\tilde{u})](\mathbf{x}, t) - J[\mathscr{L}(u)](\mathbf{y}(\mathbf{x}, t), s(\mathbf{x}, t)) \tag{270m}$$

where J is the determinant of the Jacobian of the transformation $T: \langle \mathbf{x}, t\rangle \to \langle \mathbf{y}, s\rangle$. The first term on the right of (270m) means compute $\mathscr{L}$ using $\tilde{u}$ in place of u. The second term means first compute $\mathscr{L}(u)$ and then make the change of variables. If $\delta\mathscr{L} = 0$, then $A_\Omega(\tilde{u}) = A_{T[\Omega]}(u)$ and thus u is stationary if and only if $\tilde{u}$ is stationary. Thus, if $\delta\mathscr{L} = 0$, then $\tilde{u}$ solves (270j) if u does. As we shall see, $\delta\mathscr{L} = 0$ is *not* necessary for the invariance of (270j) under the change of variables $u \to \tilde{u}$ (see Examples 3 and 4 below).

Noether's theorem expresses the fact that if one has a one-parameter family of transformations leaving A invariant, then one can find a conserved quantity for the corresponding Euler–Lagrange equation. The point of the above calculation was that $\delta\mathscr{L} = 0$ is sufficient for A to be invariant. In the following calculations one should think of $\langle \mathbf{x}, t\rangle$ ranging throughout $\mathbb{R}^{n+1}$

and all transformations being smooth. In fact, in applications one very often wishes to use singular transformations that are not defined on all of $\mathbb{R}^{n+1}$; the set of regions Ω is then restricted to stay away from the singular set. Although these subtleties cause some difficulties in theory, they do not in practice. For "Noether's theorem" is really just a clever way to organize the chain rule, and, at the end, one has in one's hand a candidate for a conserved quantity for the differential equation. The conservation can always be checked explicitly; the importance of Noether's theorem is that it sets up an organized scheme for providing candidates.

So, let

$$s_\varepsilon = s(\mathbf{x}, t, \varepsilon), \qquad \mathbf{y}_\varepsilon = \mathbf{y}(\mathbf{x}, t, \varepsilon)$$

be a smooth family of smooth coordinate changes and let V_ε be a smooth family of smooth maps from $\mathbb{R}^{n+2}$ to $\mathbb{R}$. Define

$$\tilde{u}_\varepsilon(\mathbf{x}, t) = V_\varepsilon(u(\mathbf{y}_\varepsilon, s_\varepsilon), \mathbf{y}_\varepsilon, s_\varepsilon)$$

Assume further that for $\varepsilon = 0, s_0 = t, \mathbf{y}_0 = \mathbf{x}$, and $V_0(u(\mathbf{y}_0, s_0), \mathbf{y}_0, s_0) = u$, so our change of variables, both dependent and independent, is the identity at $\varepsilon = 0$. Now, define

$$X_j(\mathbf{x}, t) = \left.\frac{\partial(\mathbf{y}_\varepsilon)_j}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad X_0(\mathbf{x}, t) = \left.\frac{\partial s_\varepsilon}{\partial\varepsilon}\right|_{\varepsilon=0}$$

$$\Psi(u, \mathbf{x}, t) = \left.\frac{\partial V_\varepsilon}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad S(u) = \left.\frac{\partial(\delta_\varepsilon\mathscr{L})}{\partial\varepsilon}\right|_{\varepsilon=0}$$

$$j_0 = (u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi)\frac{\partial\mathscr{L}}{\partial u_t} - \mathscr{L}X_0 \tag{270n}$$

$$\mathbf{j} = (u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi)\frac{\partial\mathscr{L}}{\partial(\nabla u)} - \mathscr{L}\mathbf{X} \tag{270o}$$

Then, letting $\partial_0 \equiv \partial/\partial t$:

$$\partial_0 j_0 + \nabla \cdot \mathbf{j} = S(u) \tag{270p}$$

Thus, in particular, if $\delta_\varepsilon\mathscr{L} \equiv 0$ for all ε and if $\langle j_0, \mathbf{j}\rangle$ fall off sufficiently rapidly at ∞, then $\int_{\mathbb{R}^n} j_0(x, t)\, d^n x$ is a constant. To prove (270p) we first note that

$$F \equiv \left.\frac{\partial\tilde{u}_\varepsilon}{\partial\varepsilon}\right|_{\varepsilon=0} = u_t X_0 + \nabla u \cdot \mathbf{X} + \Psi$$

So, for $\varepsilon = 0$, we can write

$$\partial_0 j_0 + \nabla \cdot \mathbf{j} = \left\{ \frac{\partial \mathscr{L}}{\partial u_t} \frac{\partial F}{\partial t} + \frac{\partial \mathscr{L}}{\partial (\nabla u)} \cdot \nabla F + \left[\frac{\partial}{\partial t}\left(\frac{\partial \mathscr{L}}{\partial u_t} \right) + \nabla \cdot \left(\frac{\partial \mathscr{L}}{\partial (\nabla u)} \right) \right] F \right\}$$
$$- \frac{\partial \mathscr{L}}{\partial t} X_0 - (\nabla \mathscr{L}) \cdot \mathbf{X} - \mathscr{L}\left(\frac{\partial X_0}{\partial t} + \nabla \cdot \mathbf{X} \right) \qquad (270q)$$

Using the Euler–Lagrange equation (270j), we recognize the quantity in $\{\cdot\}$ as $\partial \mathscr{L}(\tilde{u}_\varepsilon)/\partial \varepsilon \,|_{\varepsilon = 0}$. Moreover,

$$\frac{\partial \mathscr{L}}{\partial t} X_0 + \nabla \mathscr{L} \cdot \mathbf{X} = \frac{\partial}{\partial \varepsilon} [\mathscr{L}(\mathrm{y}, s)] \bigg|_{\varepsilon = 0}$$

and

$$\frac{\partial J}{\partial \varepsilon}\bigg|_{\varepsilon = 0} = \frac{\partial X_0}{\partial t} + \nabla \cdot \mathbf{X}$$

so that the right-hand side of (270q) can be recognized as $S(u)$. This proves (270p).

$j = \langle j_0, \mathbf{j} \rangle$ is called the **current** associated to the one-parameter family; and if $\partial_0 j_0 + \nabla \cdot \mathbf{j} = 0$, we say that the current is **conserved**. $S(u)$ is called the **source** for j.

Example 1 (conservation of energy and the energy–momentum tensor) Consider the equation $u_{tt} = \Delta u - F(u)$. Then, the Lagrangian is $\frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - G(u)$ where $G(y) = \int_0^y F(x)\, dx$. Clearly, the family of time translations $\langle \mathrm{x}, t \rangle \to \langle \mathrm{x}, t + \varepsilon \rangle$, $V_\varepsilon(u) = u$ leaves the equations of motion invariant and it is easy to see that $\delta \mathscr{L} = 0$ for all ε. Moreover, $\mathbf{X} = 0$, $\Psi = 0$, $X_0 = 1$. The resulting current, j_0, j_i, usually denoted by t_{00}, t_{0i}, is given by:

$$t_{00} = \tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + G(u), \qquad t_{0i} = -u_t(\nabla_i u)$$

It follows from (270j) that $\partial_0 t_{00} + \sum_{i=1}^n \partial_i t_{0i} = 0$ and we recognize $(d/dt) \int t_{00}\, dx = 0$ as conservation of energy (of course this can be computed directly by using the differential equation and integration by parts). The reason that one denotes the current with two indices is that one can just as well consider invariants under space translations $\langle \mathrm{x}, t \rangle \to \langle \mathrm{x} + \varepsilon \delta_i, t \rangle$ where $\delta_i = \langle 0, \ldots, 1, \ldots, 0 \rangle$ with 1 in the ith place. The resulting current j_0, j_k is usually denoted t_{i0}, t_{ik}. One finds that

$$t_{0i} = -t_{i0} \qquad \text{and} \qquad t_{ij} = t_{ji}; \qquad 1 \le i, j \le n \qquad (270r)$$

In particular, the momentum $\int u_t(\nabla_i u)\, d^n x$ is conserved. $t_{\mu\nu}$ is often called the **energy–momentum tensor**, although in fully relativistic notation, what we call $t_{\mu\nu}$ is usually called $T^{\mu}{}_{\nu}$.

Example 2 (the dilation current for (270b)) Because of the special choice of the 3 in (270b), one sees that solutions of (270b) are taken into themselves under the transformation $\langle \mathbf{x}, t\rangle \to \langle \lambda\mathbf{x}, \lambda t\rangle$; $u \to \lambda u$. For these **dilation transformations**, $\delta\mathscr{L}$ is easily seen to be zero. If we take $\lambda = e^{\varepsilon}$, then $X_0 = t$, $X_i = x_i$, $\Psi = u$. The resulting conserved quantity is

$$\int [t(\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4) + u_t \mathbf{x}\cdot\nabla u + u_t u]\, d^3x \tag{270s}$$

We have included the general form of (270p) including the source term $S(u)$ for two reasons. First the **broken invariance** occurring when $S(u) \neq 0$ can be useful; for example, if $S(u) \le 0$ for $t \ge 0$, then (270p) implies that $\int j_0(x, t)\, d^3x \le \int j_0(x, 0)\, d^3x$ for all $t \ge 0$ and this can be useful (see Problem 153). Secondly, if it happens that $S(u)$ is of the form $\partial_0 b_0 + \nabla\cdot\mathbf{b}$, then one finds that $\partial_0 k_0 + \nabla\cdot\mathbf{k} = 0$ for $\mathbf{k} = \mathbf{j} - \mathbf{b}$, so that k_0 is conserved. We shall first compute a broken symmetry and then turn to a class of cases where $S(u)$ is automatically of the form $\partial_0 b_0 + \nabla\cdot\mathbf{b}$.

Example 3 (broken dilation invariance for $u_{tt} = \Delta u - u|u|^{p-1}$) If $\mathscr{L} = \frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - (p+1)^{-1}|u|^{p+1}$ in three space dimensions, then under the dilation $\langle \mathbf{x}, t\rangle \to \langle \lambda\mathbf{x}, \lambda t\rangle$, $u \to \lambda u$, $\delta\mathscr{L}$ is not zero if $p \neq 3$. The part of $\mathscr{L}$ giving $u_{tt} - \Delta u$ is invariant, but

$$\delta\mathscr{L} = -(p+1)^{-1}(\lambda^{p+1} - \lambda^4)|u(\lambda\mathbf{x}, \lambda t)|^{p+1}$$

Taking $\lambda = e^{\varepsilon}$ and evaluating $\partial(\delta_\varepsilon\mathscr{L})/\partial\varepsilon$, one finds that

$$S(u) = (p+1)^{-1}(3-p)|u|^{p+1}$$

so that $S(u) \le 0$ for $p \ge 3$. Since the dilation charge (270s) does not have obvious positivity properties, this is of limited value; but the conformal invariance which we use to prove Theorem XI.101 can be replaced by broken conformal invariance to prove the analogous result for

$$u_{tt} = \Delta u - u|u|^{p-1} \tag{270t}$$

if $3 < p < 5$ (Problem 153). Actually, this equation has a type of dilation invariance; clearly under $\langle \mathbf{x}, t\rangle \to \langle \lambda\mathbf{x}, \lambda t\rangle$, $u \to \lambda^{\alpha}u$ with $\alpha = 2(p-1)^{-1}$, solutions of (270r) go into other solutions. It is not true that $\delta\mathscr{L} = 0$ in this case; rather $\mathscr{L}(\tilde{u}) = \lambda^{2+2\alpha}\mathscr{L}(u)(y, s)$, while $J\mathscr{L}(u)(y, s) = \lambda^{4\alpha}\mathscr{L}(u)$. This means that $A_\Omega(\tilde{u}) = \lambda^{2-2\alpha}A_{T[\Omega]}(u)$; so one can understand the invariance of the differential equation from the principle of stationary action. However $S(u) = (2 - 2\alpha)\mathscr{L}(u)$, so the current associated to this dilation transformation is not conserved. Moreover, S is not a divergence (Problem 154); so one cannot get a conserved current by changing from j to k. This shows that an invariance of the differential equation that is not a strict invariance of the action may not lead to a new conserved quantity.

There is one general case where $S(u)$ is automatically of the form $\partial_0 b_0 + \nabla \cdot \mathbf{b}$, namely if $\delta_\varepsilon \mathscr{L} = \partial_0 B_0^{(\varepsilon)} + \nabla \cdot \mathbf{B}^{(\varepsilon)}$; for take $b_0 = \partial B_0^{(\varepsilon)}/\partial\varepsilon$, $\mathbf{b} = \partial \mathbf{B}^{(\varepsilon)}/\partial\varepsilon$. Notice that if

$$\delta\mathscr{L} = \partial_0 B_0 + \nabla \cdot \mathbf{B} \tag{270u}$$

where $B(\mathbf{x})$ is a function only of $\tilde{u}$ and its derivatives at $\mathbf{x}$, then $A_\Omega(\tilde{u}) = A_{T(\Omega)}(u) + \int_{\partial\Omega} B_0\, d\sigma_0 + \mathbf{B} \cdot d\boldsymbol{\sigma}$, so that for $\tilde{v}$'s vanishing near $\partial\Omega$,

$$A_\Omega(\tilde{u} + \lambda\tilde{v}) - A_\Omega(\tilde{u}) = A_{T(\Omega)}(u + \lambda v) - A_{T[\Omega]}(u)$$

Thus (270p) implies that the transformation takes solutions of the Euler–Lagrange equations into other solutions. When $S(u) = \partial_0 b_0 + \nabla \cdot \mathbf{b}$, $\int (j_0 - b_0)\, d^n x$ is conserved, so that invariance of the basic differential equations may be connected with a conserved quantity different from $\int j_0\, d^n x$.

Example 4 (conformal invariance of (270b)) The inversion $z \to z^{-1}$ is analytic in the complex plane away from zero; so $u(x(x^2 + y^2)^{-1}, -y(x^2 + y^2)^{-1})$ is harmonic on $\mathbb{R}^2\backslash\{0\}$ if u is. Formal continuation from x to ix suggests that if $u_{tt} - u_{xx} = 0$, then $u(x(t^2 - x^2)^{-1}, t(t^2 - x^2)^{-1})$ also solves the wave equation away from $t^2 - x^2 = 0$, and this can be seen from straightforward calculation. In four dimensions this is no longer true; to see this consider the harmonic case first. $u(\mathbf{x}) = |\mathbf{x}|^{-2}$ is harmonic away from $\mathbf{x} = \mathbf{0}$, but $\tilde{u}(\mathbf{x}) \equiv u(\mathbf{x}|\mathbf{x}|^{-2}) = |\mathbf{x}|^2$ is not. Since the only other radially symmetric function that is harmonic is 1, one might try $\tilde{u}(\mathbf{x}) \equiv |\mathbf{x}|^{-2}u(\mathbf{x}|\mathbf{x}|^{-2})$; and, indeed, one can show by tedious calculation that $\Delta\tilde{u} = |\mathbf{x}|^{-4}(\Delta u)^\sim$. Similarly, for $\mathbf{x} \in \mathbb{R}^3$, $t \in \mathbb{R}$, we define the **Lorentz inversion** by

$$\mathbf{y}(t, \mathbf{x}) = \mathbf{x}(t^2 - |\mathbf{x}|^2)^{-1}, \qquad s(t, \mathbf{x}) = t(t^2 - |\mathbf{x}|^2)^{-1}$$

$$V(u, \mathbf{x}, t) = (t^2 - |\mathbf{x}|^2)^{-1}u$$

If $\tilde{u}(\mathbf{x}, t) = V(u(\mathbf{y}, s), \mathbf{y}, s)$, then $\tilde{u}$ solves $u_{tt} = \Delta u$ if and only if u does. Indeed

$$\tilde{u}_{tt} - \Delta\tilde{u} = (t^2 - |\mathbf{x}|^2)^{-2}(u_{tt} - \Delta u)^\sim \tag{270v}$$

Since the transformations are singular when $|\mathbf{x}| = t$, this is true only away from $|\mathbf{x}| = t$. We shall not explicitly worry about this problem below, but we note that we only show directly that $\partial_0 k_0 + \nabla \cdot \mathbf{k} = 0$ for points $\langle \mathbf{x}, t \rangle$ with $|\mathbf{x}| \neq t$ when k_0 and $\mathbf{k}$ are given by (270d) and (270i). However, k_0 and $\mathbf{k}$ are easily seen to be C^∞; so the result holds for all $\langle \mathbf{x}, t \rangle$ and therefore one obtains conservation of the conformal charge $\int k_0 \, d^3x$.

(270v) shows that $u \to \tilde{u}$ also preserves solutions of (270b). This suggests that we compute the change $\delta\mathcal{L}$ under the Lorentz inversion for the Lagrangian $\mathcal{L} = \frac{1}{2}u_t^2 - \frac{1}{2}(\nabla u)^2 - \frac{1}{4}u^4$. For this calculation, it is convenient to shift to relativistic notation: Let x_μ ($\mu = 0, 1, 2, 3$) be t, x_1, x_2, x_3, and x^μ be $t, -x_1, -x_2, -x_3$. Define $g^{\mu\nu} = g_{\mu\nu}$ to be the matrix that is zero if $\mu \neq \nu$ and that is 1 (respectively, -1) if μ and ν have the common value 0 (respectively, 1, 2, or 3). Finally, let $\partial^\mu = \partial/\partial x_\mu$. Also, we shall use the summation convention, i.e., $x^\lambda x_\lambda = t^2 - |x|^2$, $\partial^\lambda \partial_\lambda = \partial_0^2 - \Delta$, etc. We begin by looking at the Jacobian matrix $T^\mu{}_\nu = \partial^\mu y_\nu$ where $y_\nu = (x^\lambda x_\lambda)^{-1} x_\nu$ is the Lorentz inversion. By direct calculation $T^\mu{}_\nu = (x^\lambda x_\lambda)^{-1} S^\mu{}_\nu$ where

$$S^\mu{}_\nu = \delta^\mu{}_\nu - 2(x^\lambda x_\lambda)^{-1} x^\mu x_\nu \tag{270w}$$

and $\delta^\mu{}_\nu$ is the unit matrix. The point is that $S^\mu{}_\nu$ is a Lorentz transformation, i.e.,

$$S^\lambda{}_\kappa g_{\lambda\mu} S^\mu{}_\nu = g_{\kappa\nu}$$

Taking determinants, we see that $|\det(S)| = 1$, so that the Jacobian $J = |\det(T)| = (x^\lambda x_\lambda)^{-4}$. Using the above invariance,

$$g_{\mu\nu} T^\mu{}_\kappa T^\nu{}_\lambda \, \partial^\kappa v \, \partial^\lambda v = (x^\lambda x_\lambda)^{-2} g_{\mu\nu} \, \partial^\mu v \, \partial^\nu v \tag{270x}$$

Now let $\tilde{u}(x) \equiv (x^\lambda x_\lambda)^{-1} u(y(x))$. Then

$$\partial^\mu \tilde{u} = (x^\lambda x_\lambda)^{-1} T^\mu{}_\nu (\partial^\nu u)(y) - 2(x^\lambda x_\lambda)^{-2} x^\mu u(y) \tag{270y}$$

If one now uses (270x) and $\mathcal{L}(u) = \frac{1}{2} g_{\mu\nu} \, \partial^\mu u \, \partial^\nu u - \frac{1}{4}u^4$, one sees that

$$\begin{aligned}(\delta\mathcal{L})(u) &= 2(x^\lambda x_\lambda)^{-3} u(y)^2 - 2(x^\lambda x_\lambda)^{-3} x_\mu u \, \partial^\mu(u(y)) \\ &= \partial_\mu B^\mu \end{aligned} \tag{270z}$$

where $B^\mu = -x^\mu (x^\lambda x_\lambda)^{-3} u(y)^2$. The terms in (270z) come from squaring (270y) and using the fact that only the square of the $\partial^\mu u$ term in $\mathcal{L}(\tilde{u})$ is cancelled by a term in $J\mathcal{L}(u)(y)$.

Lorentz inversion is not a continuous symmetry, but a single transformation. However, if we invert, then translate by $-\varepsilon$ in time, and then invert, we do get a continuous group of symmetries. Thus, we define:

$$\mathbf{y}(\mathbf{x}, t, \varepsilon) = \mathbf{x}F, \qquad s(\mathbf{x}, t, \varepsilon) = (t - \varepsilon(t^2 - |\mathbf{x}|^2))F$$

$$V(\mathbf{x}, t, u, \varepsilon) = uF$$

$$F(\mathbf{x}, t, \varepsilon) = (t^2 - |\mathbf{x}|^2)[\{t - \varepsilon(t^2 - |\mathbf{x}|^2)\}^2 - |\mathbf{x}|^2]^{-1}$$

This rather complicated expression is called a conformal transformation. More properly, the conformal group is the 15 parameter group of Poincaré transformations, dilations, and the conjugation of space-time translations by Lorentz inversion. Correspondingly, there are 15 conserved quantities for (270b) of which we use only two (the energy and the time component of the conformal charge) to prove Theorem XI.101, although we have also considered the momentum (three components) and dilations in this appendix.

For the above conformal transformation, we have that $\Psi = 2tu$, $X_j = 2x_j t$, $X_0 = t^2 + |\mathbf{x}|^2$ by straightforward differentiation. Thus

$$j_0 = (|x|^2 + t^2)(\tfrac{1}{2}u_t^2 + \tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{4}u^4) + 2tu_t \mathbf{x} \cdot \nabla u + 2tu_t u$$

$$\mathbf{j} = (-\nabla u)\{(|\mathbf{x}|^2 + t^2)u_t + 2t\mathbf{x} \cdot \nabla u + 2tu\} - 2t\mathbf{x}(\tfrac{1}{2}u_t^2 - \tfrac{1}{2}(\nabla u)^2 - \tfrac{1}{4}u^4)$$

Given that $\delta\mathscr{L}$ is not zero for the inversion, we do not expect this for the conformal map either; but we do expect that $S(u) = \partial^\mu b_\mu$ since $\delta\mathscr{L} = \partial^\mu B_\mu$ for an inversion. As in the calculation of the inversion, $S(u)$ comes from the difference of $\frac{1}{2}(\partial^\mu \tilde{u})(\partial_\mu \tilde{u})$ and $\frac{1}{2}J(\partial^\mu u)(\partial_\mu u)$. Since

$$\tilde{u} = (1 + 2\varepsilon t)u(y) + O(\varepsilon^2)$$

we have that

$$\partial^\mu \tilde{u} = (1 + 2\varepsilon t)\partial^\mu(u(y)) + 2\varepsilon\delta^\mu{}_0 u + O(\varepsilon^2)$$

so the extra term is (up to $O(\varepsilon^2)$) just $\frac{1}{2}[4\varepsilon\delta^\mu{}_0 u(\partial^\mu u)] = \varepsilon\partial_0(u^2)$. Thus $S(u) = \partial_0(u^2)$ and therefore, if we set $\mathbf{k} = \mathbf{j}$, $k_0 = j_0 - u^2$, then $\partial_0 k_0 + \nabla \cdot \mathbf{k} = 0$. We have therefore verified that for (270b), the charge given by (270c) is conserved. More importantly, we have described how to find such conserved quantities.

XI.14 Spin wave scattering

We want to discuss a physical system that is very different from those we have discussed so far but whose scattering structure is well described by the two Hilbert space formalism we introduced in Section 3. We consider a system of quantum mechanical spins, one at each lattice point of $\mathbb{Z}^3 \subset \mathbb{R}^3$, each interacting with its nearest neighbors. The basic states for each spin are "spin-up" and "spin-down"; but since the system is quantum mechanical, we must allow superpositions. Thus the set of states for a single spin at a fixed site $\alpha \in \mathbb{Z}^3$ is the unit sphere in a two-dimensional complex Hilbert space. If we have, at time $t = 0$, a state where one given spin is up and all the others are down, then the interactions, which we describe precisely below, are such that as the system evolves a "wave" of single spin-up states propagates through the system, that is, a time-dependent superposition of states with one spin up results with more and more weighting of sites far from the initial spin as $t \to \infty$. If we started initially with two spins up, then a superposition of states of two spins up results. If the two spins are far from one another initially, then for very small times the two spins propagate more or less as two independent single spin waves because the interactions are nearest neighbor. As they move in time, these will develop nonzero probabilities of being in a state with two neighboring spins up, which then interact and scatter. It is this process we want to describe.

This system of spins is a model (called the **Heisenberg model**) of a ferromagnet. The spins have magnetic moments and the basic interaction is magnetic. The excitations we described above are usually called **magnetic spin waves** or **magnons**. One feature to note in our system is that we have considered the spin waves in a background of all down spins, which as we shall see corresponds to a ground state of the system. One could just as well consider a system with all spins up or all spins in a fixed direction which are other possible ground states. In fact, because of an overall rotational symmetry, such theories are equivalent to the one we develop. It is only at zero absolute temperature that a system will be in a ground state; at higher temperatures one has a "superposition of excited states." There has been some deep nonrigorous work on magnons at nonzero temperatures (see the Notes).

Our discussion in this section is related to various topics which we have not yet discussed. First, we are dealing with an infinite system; and, in general, infinite systems are described most naturally in the language of C^*-algebras. This is true of the Heisenberg model at nonzero temperatures; but because one can explicitly describe the ground state of the Heisenberg magnet, one is able to avoid C^*-algebraic machinery in this case. Even here, there are other ideas that are physically and mathematically interesting, such as the phenomenon of spontaneously broken symmetry, which require C^*-algebras. We return to these ideas in later volumes. Secondly, all the scattering situations we have described thus far involve the comparison of an a priori "free dynamics" with the interacting system. In our current situation the "free dynamics" is not given by some a priori comparison system but rather by a piece of the interacting system, namely the dynamics of the one magnon states. This idea will reoccur in our study of interacting quantum field scattering in Section 16.

We first describe the model for finitely many spins. Let Λ be a finite subset of $\mathbb{Z}^3$. To each $\alpha \in \Lambda$ we associate a copy of $\mathbb{C}^2$, call it $\mathbb{C}^2_\alpha$. We refer to the vectors

$$e_1^{(\alpha)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad e_0^{(\alpha)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

respectively as the **spin up** and **spin down** states at α. The Hilbert space for finitely many spins $\mathscr{H}_\Lambda$, one at each point of Λ, is

$$\mathscr{H}_\Lambda = \bigotimes_{\alpha \in \Lambda} \mathbb{C}^2_\alpha \tag{271}$$

The set of vectors of the form $\bigotimes_{\alpha \in \Lambda} e_{a_\alpha}^{(\alpha)}$, where $\{a_\alpha\}_{\alpha \in \Lambda}$ is a sequence of zeros and ones, is a basis for $\mathscr{H}_\Lambda$; for notational convenience, we set $\psi(\{a_\alpha\}) \equiv \bigotimes_{\alpha \in \Lambda} e_{a_\alpha}^{(\alpha)}$.

In order to define the Hamiltonian H_Λ for the finite system we need some terminology. Let σ_x, σ_y, σ_z denote the Pauli matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and set $\sigma_\pm \equiv \frac{1}{2}(\sigma_x \pm i\sigma_y)$ so that

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

σ_+ flips a down spin up, and σ_- flips an up spin down. That one can think of $\frac{1}{2}\boldsymbol{\sigma}$ as the three components of a quantum angular momentum follows from the fact that they obey the commutation relations of the Lie algebra of the three-dimensional rotation group. For each $\alpha \in \Lambda$, we denote by $\sigma_x^{(\alpha)}$, $\sigma_y^{(\alpha)}$, $\sigma_z^{(\alpha)}$, $\sigma_\pm^{(\alpha)}$ the operator on $\mathscr{H}_\Lambda$ which acts (respectively) by σ_x, σ_y, σ_z, $\sigma_\pm$ on the α component of the tensor product and by the identity on the other components. Thus, in terms of the basis $\psi(\{a_\beta\})$,

$$\sigma_z^{(\alpha)}\psi(\{a_\beta\}) = (2a_\alpha - 1)\psi(\{a_\beta\})$$

$$\sigma_+^{(\alpha)}\psi(\{a_\beta\}) = \begin{cases} 0, & \text{if} \quad a_\alpha = 1 \\ \psi(\{a_\beta + \delta_{\beta\alpha}\}), & \text{if} \quad a_\alpha = 0 \end{cases}$$

The Hamiltonian is then defined by

$$H_\Lambda = -\frac{1}{2} \sum_{\substack{|\alpha - \beta| = 1 \\ \alpha,\, \beta \in \Lambda}} (\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 4\sigma_+^{(\alpha)}\sigma_-^{(\beta)}) \tag{272}$$

The sum runs over all nearest-neighbor *ordered* pairs $\langle\alpha, \beta\rangle$. Because of the factor $\frac{1}{2}$, each unordered pair contributes an energy $\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 2\sigma_+^{(\alpha)}\sigma_-^{(\beta)} + 2\sigma_-^{(\alpha)}\sigma_+^{(\beta)} = \boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)}$ where we have set $\boldsymbol{\sigma}^{(\alpha)} = \langle\sigma_x^{(\alpha)}, \sigma_y^{(\alpha)}, \sigma_z^{(\alpha)}\rangle$. Given the connection with rotations mentioned above, the basic interaction Hamiltonian can be seen to be invariant under simultaneous rotations of all the spins. The minus sign of (272) means that states with spins parallel to each other tend to have lower energy than those antiparallel.

It can be shown (Problem 132) that if the set Λ becomes a connected set when nearest neighbors are joined, then the ground state for H_Λ is $(n + 1)$-degenerate where n is the number of points in Λ. The ground state has energy $-k$ where k is the number of nearest-neighbor pairs. One of the ground state eigenvectors is $\psi_0 \equiv \bigotimes_{\alpha \in \Lambda} e_0^{(\alpha)}$. The rest of a basis of ground state eigenvectors may be obtained by applying the operator $\sum_{\alpha \in \Lambda} \sigma_+^{(\alpha)}$ some number of times.

There are two difficulties in dealing with the case $\Lambda = \mathbb{Z}^3$. First, we must decide what to take for the Hilbert space of the infinite volume system. Secondly, we must decide what to take for the Hamiltonian, especially in view of the fact that the ground state energy (that is, lowest eigenvalue) of H_Λ goes to $-\infty$ as $|\Lambda|$, the volume of Λ, goes to infinity.

One method of defining the infinite volume Hilbert space is to develop the idea of infinite tensor product and use (271); but since we shall primarily be interested in a different realization of the basic structure, we defer discussion of infinite tensor products to the Notes. We consider an infinite-dimensional Hilbert space $\mathscr{H}$ with basis $\{\psi(\{a_\beta\})\}$ where $a = \{a_\beta\}$ is a sequence of zeros and ones indexed by $\mathbb{Z}^3$ *with only finitely many* $a_\beta \neq 0$; that is, $\mathscr{H}$ consists of vectors of the form

$$\sum_a{}' \, c(a)\psi(a)$$

($\sum'$ means we allow a's only with the above italicized restriction) where $c(a) \in \mathbb{C}$ and $\sum_a' |c(a)|^2 < \infty$. The inner product on $\mathscr{H}$ is given by

$$\left(\sum{}' d(a)\psi(a), \sum{}' c(a)\psi(a)\right) = \sum{}' \overline{d(a)}c(a)$$

ψ_0 will stand for the basis vector where all the a_β are chosen equal to zero.

A complete justification for taking this Hilbert space in the infinite volume limit requires the C^*-algebraic approach, but we note that without the italicized condition the constructed Hilbert space would be inseparable while $\mathscr{H}$ is separable. Moreover, we can define $\sigma_x^{(\alpha)}$, $\sigma_y^{(\alpha)}$, $\sigma_z^{(\alpha)}$, $\sigma_\pm^{(\alpha)}$ as before and we can define a Hamiltonian H, as we shall see.

One cannot use (271) to define $H_{\mathbb{Z}^3}$ since on each $\psi(\{a_\beta\})$ the sum is divergent. However, if we replace $\sigma_z^{(\alpha)}\sigma_z^{(\beta)}$ by $\sigma_z^{(\alpha)}\sigma_z^{(\beta)} - 1$ whenever it occurs, that is, we define

$$H_{\mathbb{Z}^3} = -\tfrac{1}{2} \sum_{\substack{|\alpha-\beta|=1 \\ \alpha,\beta\in\mathbb{Z}^3}} \left(\sigma_z^{(\alpha)}\sigma_z^{(\beta)} - 1 + 4\sigma_+^{(\alpha)}\sigma_-^{(\beta)}\right) \tag{273}$$

then the sum converges on each $\psi(\{a_\beta\})$. Since we have just changed the ground state energy by a (infinite) constant, the physics should be the same. We now drop the $\mathbb{Z}^3$ and take the domain of H, $D(H)$, to be the dense set of finite linear combinations of the vectors $\psi(a)$. Since for each vector v in $D(H)$ all but finitely many terms of Hv are zero, H is well defined on $D(H)$. In fact:

Proposition H is essentially self-adjoint and nonnegative. ψ_0 is the unique vector with $H\psi_0 = 0$.

Proof Let $\mathscr{H}_n$ be the span of those $\psi(\{a_\beta\})$ with $\sum_\beta a_\beta = n$. Then $\mathscr{H} = \bigoplus \mathscr{H}_n$, $\mathscr{H}_n \subset D(H)$, H leaves $\mathscr{H}_n$ invariant, and H is bounded on each $\mathscr{H}_n$. It follows that H is a direct sum of bounded self-adjoint operators and so is essentially self-adjoint by an elementary argument we have used often before (see Example 2 in Section VIII.10 or Problem 1 of Chapter X). H is positive because

$$\sigma_z^{(\alpha)}\sigma_z^{(\beta)} + 2\sigma_+^{(\alpha)}\sigma_-^{(\beta)} + 2\sigma_-^{(\alpha)}\sigma_+^{(\beta)} \le 1$$

for any α and β (Problem 131). The simplicity of the zero eigenvalue is left to the problems (Problem 133). ▮

As we have mentioned in the last proof, H leaves each subspace $\mathscr{H}_n$ invariant. Let us begin by analyzing $H \restriction \mathscr{H}_1$. For each $\alpha \in \mathbb{Z}^3$, let $\eta_\alpha = \psi(\{\delta_{\alpha\beta}\})$, that is, η_α is the vector describing the state with spin up at site α and spin down at all other sites. By definition of H and the fact that α has six nearest neighbors β_i occurring as both (α, β_i) and (β_i, α) in the sum (273),

$$H\eta_\alpha = 12\eta_\alpha - 2 \sum_{|\beta-\alpha|=1} \eta_\beta$$

An arbitrary $\varphi \in \mathscr{H}_1$ can be expanded

$$\varphi = \sum_{\alpha\in\mathbb{Z}^3} \varphi(\alpha)\eta_\alpha$$

so $H\varphi = \sum (H\varphi)(\alpha)\eta_\alpha$ where

$$(H\varphi)(\alpha) = 2\left(6\varphi(\alpha) - \sum_{|\beta-\alpha|=1} \varphi(\beta)\right) \tag{274}$$

To better understand $H \upharpoonright \mathscr{H}_1$, notice that H commutes with the obvious representation of $\mathbb{Z}^3$ as translations on $\mathscr{H}$. Thus, the map of $\ell^2(\mathbb{Z}^3)$ given by $\{\varphi(\alpha)\} \mapsto \{(H\varphi)(\alpha)\}$ commutes with translations, as is obvious from (274). Thus the Fourier transform $\ell^2(\mathbb{Z}^3) \overset{\frown}{\to} L^2([-\pi, \pi]^3)$ should give a spectral representation for H. Indeed, defining

$$\hat{\varphi}(k) = (2\pi)^{-3/2} \sum_{\alpha \in \mathbb{Z}^3} \varphi(\alpha) e^{-ik \cdot \alpha}$$

we find that

$$(\widehat{H\varphi})(k) = \mu(k)\hat{\varphi}(k)$$

where

$$\mu(k) = 4(3 - \cos k_1 - \cos k_2 - \cos k_3)$$

Thus $H \upharpoonright \mathscr{H}_1$ looks much like a lattice version of the free kinetic energy in nonrelativistic quantum mechanics since for k small, $\mu = 2|k|^2 + O(k^4)$.

We can now describe the sense in which $H \upharpoonright \mathscr{H}_2$ is a Hamiltonian describing states that look asymptotically like two single spin waves moving freely. First we need to note that the natural two spin-wave space is not $\mathscr{H}_2$ but rather $\mathscr{H}_1 \otimes_s \mathscr{H}_1$. The reason for the symmetric tensor product is that, physically, it makes no sense to say which of the two up spins is "first." The reason for symmetry is that we have chosen the spin operators at different sites to commute, a choice based on the fact that these spins should be independent observable quantities. Had we taken the σ's to anticommute, we would have obtained a "free Fermi gas" without any scattering.

We define

$$J_2 \colon (\mathscr{H}_1 \otimes_s \mathscr{H}_1) \to \mathscr{H}_2$$

$$J_2(\eta_\alpha \otimes_s \eta_\gamma) = \begin{cases} \psi(\{\delta_{\alpha\beta} + \delta_{\gamma\beta}\}), & \alpha \neq \gamma \\ 0, & \alpha = \gamma \end{cases}$$

and use the two Hilbert space scattering theory of Section 3.

Theorem XI.102 Let $H_2 \equiv H \upharpoonright \mathscr{H}_2$ and $H_1^\otimes = H_1 \otimes I + I \otimes H_1$. Then

$$\Omega_2^\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{+itH_2} J_2 e^{-itH_1^\otimes}$$

exist and are isometries of $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ into $\mathscr{H}_2$.

Proof By Cook's method, the limit exists if we can prove that

$$\int_{\pm 1}^{\pm\infty} \|[H_2 J_2 - J_2 H_1^\otimes] e^{-itH_1^\otimes} \varphi\| \, dt < \infty \tag{275}$$

for a total set of φ's. Moreover, to prove that $\Omega_2^\pm$ are isometries, we need only show that

$$\|(J_2^* J_2 - 1)e^{-itH_1^\otimes}\varphi\| \to 0 \tag{276}$$

as $t \to \pm\infty$. We shall prove (275) and leave (276) to the reader (Problem 134).

Let us define $V: \mathscr{H}_1 \otimes_s \mathscr{H}_1 \to \mathscr{H}_1 \otimes_s \mathscr{H}_1$ by

$$V = J_2^* H_2 J_2 - H_1^\otimes$$

V has two important properties. First, it is bounded. Secondly, V has support in the region $|\alpha - \beta| \le 2$ in the following sense. Identify $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ with the symmetric functions in $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ by the map $\varphi \mapsto \tilde{\varphi}(\cdot, \cdot)$ where $\varphi = \sum \tilde{\varphi}(\alpha, \beta)\eta_\alpha \otimes \eta_\beta$. Define $\tilde{V}$ by $\tilde{V}\tilde{\varphi} = \widetilde{V\varphi}$. If we define an operator χ on $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ by

$$(\chi\tilde{\varphi})(\alpha, \beta) = \begin{cases} \tilde{\varphi}(\alpha, \beta), & \text{if } \ |\alpha - \beta| \le 2 \\ 0, & \text{if } \ |\alpha - \beta| > 2 \end{cases}$$

then $\tilde{V}\chi = \tilde{V}$. This follows by noting that H_2 acts just like $H_1^\otimes$ as long as α and β are not nearest neighbors and do not have a neighbor in common. From now on we drop the $\tilde{}$.

Since V is so nice, we shall obtain (275) by a simple application of stationary phase ideas. Denote by $\hat{}$ the Fourier transform from $\ell^2(\mathbb{Z}^3 \times \mathbb{Z}^3)$ to $L^2([-\pi, \pi]^3 \times [-\pi, \pi]^3)$. Let φ be a vector in $\mathscr{H}_1 \otimes_s \mathscr{H}_1$ such that $\hat{\varphi} \in C_0^\infty([-\pi, \pi]^3 \times [-\pi, \pi]^3)$ and:

(i) supp $\hat{\varphi}$ does not contain any point any of whose coordinates is $\pm\pi$.
(ii) supp $\hat{\varphi} \subset \{\langle k, \ell\rangle \mid \partial\mu(k)/\partial k \ne \partial\mu(\ell)/\partial\ell\}$

Then we claim that for any $m > 0$, there are constants C_m and T so that for $t > T$,

$$|(e^{-itH_1^\otimes}\varphi)(\alpha, \beta)| \le C_m(|\alpha| + |\beta| + |t| + 1)^{-m} \tag{277}$$

in the region $|\alpha - \beta| \le 2$. For the moment, assume (277). Then, for φ as above,

$$\begin{aligned} \|J_2 V e^{-itH_1^\otimes}\varphi\|_{\mathscr{H}_2}^2 &\le \|V e^{-itH_1^\otimes}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &= \|V\chi e^{-itH_1^\otimes}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &\le \|V\|^2 \|\chi e^{-itH_1^\otimes}\varphi\|_{\mathscr{H}_1 \otimes \mathscr{H}_1}^2 \\ &= \|V\|^2 \sum_{|\alpha - \beta| \le 2} |(e^{-itH_1^\otimes}\varphi)(\alpha, \beta)|^2 \\ &\le d\|V\|^2(1 + |t|)^{-4} \end{aligned}$$

by (277). Thus

$$\int_{\pm 1}^{\pm\infty} \|J_2 V e^{-itH_1^{\otimes}} \varphi\| \, dt < \infty$$

so, since $J_2 J_2^* = I$, we conclude that (275) holds. Since the set of such φ's are dense, the wave operators exist.

The proof of (277) is a simple exercise in the stationary phase machinery of the first appendix to Section 3; in fact only the elementary Theorem XI.14 is necessary. For, let $\omega = |\alpha| + |\beta| + |t|$ and

$$f_{\alpha,\beta,t}(k, \ell) = (\alpha \cdot k + \beta \cdot \ell - t\mu(k) - t\mu(\ell))(|\alpha| + |\beta| + |t|)^{-1}$$

Then

$$(e^{-itH_1^{\otimes}} \varphi)(\alpha, \beta) = \text{const} \int e^{i\omega f_{\alpha,\beta,t}(k,\ell)} \hat{\varphi}(k, \ell) \, dk \, d\ell$$

obeys (277) by Theorem XI.14 and the conditions (i) and (ii). ▮

There is little problem in extending the above ideas to n-spin waves; we use notation allowing all n at once. Let $\mathscr{F}_1$ be the Fock space built on $\mathscr{H}_1$. One defines

$$J: \mathscr{F}_1 \to \mathscr{H}$$

by mapping $\otimes_s^n \mathscr{H}_1$ onto $\mathscr{H}_n$ via

$$J(\eta_{\alpha_1} \otimes \cdots \otimes \eta_{\alpha_n}) = \begin{cases} \psi(\{\delta_{\alpha_1\beta} + \cdots + \delta_{\alpha_n\beta}\}), & \text{all } \alpha\text{'s unequal} \\ 0, & \text{otherwise} \end{cases}$$

Then, by mimicking the above proof, one easily sees that:

Theorem XI.103

$$\Omega^\pm = \operatorname*{s-lim}_{t \to \mp\infty} e^{itH} J e^{-it\,d\Gamma(H_1)}$$

exist and are isometries.

If $\varphi \in \otimes_s^n \mathscr{H}_1$, then $\Omega^\pm \varphi$ are states that asymptotically look like n free spin waves. We have just defined scattering states corresponding to a system with n spins flipped decaying into n pieces. Motivated by the N-body Schrödinger case, one can ask if there are not other channels corresponding to bound clusters of some of the flipped spins. There are, but these "bound states" have an additional complexity not present in the Schrödinger case. In the latter case the center of mass motion factors out of the full Hamiltonian, so that "bound states" are eigenvectors of a fixed operator. The key fact there is that if $\mu_S(\mathbf{k}) = k^2$, and $\sum_1^N \mathbf{k}_i = 0$, then

$$\sum_{i=1}^{N} \mu_S(\mathbf{a} + \mathbf{k}_i) = f(\mathbf{a}) + \sum_{i=1}^{N} \mu_S(\mathbf{k}_i)$$

so, for arbitrary $\mathbf{k}_i$, $\sum_{i=1}^N \mu_S(\mathbf{k}_i)$ is the sum of one function of $\mathbf{K} = \mathbf{k}_1 + \cdots + \mathbf{k}_N$ alone and one function of $\mathbf{k}_1 - \mathbf{k}_2, \ldots, \mathbf{k}_{N-1} - \mathbf{k}_N$, alone. This fails for the function $\mu(\mathbf{k}) = 3 - \cos k_1 - \cos k_2 - \cos k_3$. "Removing the center of mass motion" in a spin wave system corresponds then to realizing $H_n \equiv H \restriction \mathscr{H}_n$ as

$$(H_n \varphi)(K, k_1, \ldots, k_{n-1}) = (H_n(K)\varphi_K)(k_1, \ldots, k_{n-1})$$

where $K = k_1 + \cdots + k_n$ and $H_n(K)$ is a K-dependent operator. H_n is realized as a "fibered operator" in the sense to be discussed in Section XIII.16, or in another parlance as a "direct integral." K is the total momentum which commutes with H_n. A "bound state" is then an eigenvalue of $H_n(K)$ for some fixed K which typically varies continuously as K varies. When such "bound states" are present (and they are in the system discussed above; see the Notes), one can construct additional wave operators for the associated channels as in the Schrödinger case.

One can prove asymptotic completeness of scattering on $\mathscr{H}_2$ (Problem 135).

XI.15 Quantum field scattering I: The external field

You might think that this is a question that could be asked seriously only by a field theorist driven mad by spending too many years in too few dimensions. *S. Coleman*

In this section and the next we discuss scattering in quantum field theory. In Section 16 we show that in a field theory that satisfies the Wightman axioms and certain additional hypotheses, there is a natural way to construct a scattering operator. This general theory, called the Haag–Ruelle theory, is both elegant and important since it shows conceptually how the Wightman fields are related to the scattering of individual particles. Unfortunately, the construction of dynamics for nontrivial field theories and the verification of the Wightman axioms is very difficult and so far has been accomplished only for models in one and two space dimensions. In this section we discuss what should be a much simpler problem, scattering in an external field. This problem should be simpler because the interacting field satisfies a *linear* wave equation, for example,

$$\varphi_{tt}(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t) \qquad (278)$$

where $V(x, t)$ is the external potential.

One important phenomenon associated with the quantized version of (278) is the phenomenon of pair creation. If one starts initially with a no particle state, the expectation value of the field will be nonzero; and, as a result, because of the linearity of (278) the right-hand side will act as a source term and be nonzero. That is, there will be a nonzero probability that pairs of particles will be produced.

The phenomenon of pair creation has two striking consequences in the mathematical structure of the theory. First, the "free" dynamics at $t = -\infty$ will be different from the "free" dynamics at $t = +\infty$. Secondly, the theory is complicated in that there must be scattering amplitudes which describe the scattering of n incoming particles into m outgoing particles. It turns out that all these amplitudes can be described in terms of a certain fundamental solution of the *classical* field equation.

Before beginning the discussion of (278), we would like to describe some of the reasons external field problems are interesting. First, because external field problems are "explicitly solvable," they have often been used as approximations to and as a guide for understanding fully interacting cases. One place where the approximation has been used is in nuclear physics where the nucleon field is treated as an external field for the mesons. This is thought to be reasonable because the nucleons are so much heavier than the mesons. A place where external field problems have been used as a guide is the treatment of infrared problems in quantum electrodynamics. Secondly, certain Yukawa fields can be expressed as integrals over external fields after the fermions "have been integrated out." The external fields in this problem are not smooth and reflect the ultraviolet difficulties. Thirdly, there are a large number of invariant wave equations to choose from in the case of higher spin as well as a variety of couplings, and one would like to know which of the associated free fields are stable under coupling to an external field. If the free fields are unstable under external field coupling (that is, if the coupled theory has various pathologies), then one presumes that coupling to a fully quantized interacting field would be even worse. What is becoming apparent is that there are *no* equations of spin $\frac{3}{2}$ or greater that possess completely nonpathological external field couplings. This is not necessarily a disaster since particles of spin $\frac{3}{2}$ can arise in theories where the fields have spin $\frac{1}{2}$ (see the Notes to Section IX.8). More serious is the problem that the gravitational field in Einstein's equations has spin 2. Two ways out of this dilemma have been suggested: One is that the gravitational equations have very special nonlinearities which may not be well modeled by external fields. A more spectacular speculation is that the graviton might be a bound state of two photons and the "gravitational field"—a derived object!

In this section we shall consider only the spin zero case with the coupling (278). We assume that $V(x, t)$ is a C^∞ real-valued function of x and t with compact support. Our aim is to construct a quantum field satisfying (278) and all the Wightman axioms except Poincaré invariance (we cannot expect Poincaré invariance to hold since V is not Poincaré invariant) and then to develop a scattering theory. The great advantage of having a linear equation of motion for the field is that we can use the analogous classical wave equation to generate the quantum field dynamics. Thus we begin by studying the existence and scattering theory for the classical wave equation

$$\begin{aligned} w_{tt} - \Delta w + m^2 w &= V(x, t)w \qquad (279)\\ w(x, 0) &= w_1(x) \\ w_t(x, 0) &= w_2(x) \end{aligned}$$

As in Section 10, we set $B = \sqrt{-\Delta + m^2}$ and rewrite (279) as a first-order system

$$\frac{d}{dt}\begin{pmatrix} w \\ w_t \end{pmatrix} = \begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}\begin{pmatrix} w \\ w_t \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ V & 0 \end{pmatrix}\begin{pmatrix} w \\ w_t \end{pmatrix}$$

To make the later transition to the field theory problem easy, it is convenient to diagonalize the free part of the dynamics in the following way. Let

$$T = \frac{1}{\sqrt{2}}\begin{pmatrix} B^{1/2} & iB^{-1/2} \\ B^{1/2} & -iB^{-1/2} \end{pmatrix}$$

We set $\mathscr{h} = L^2(\mathbb{R}^3)$, take $\mathscr{h} \oplus \mathscr{h}$ as our Hilbert space, and define operators h_0 and $v(t)$ by

$$-ih_0 \equiv T\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}T^{-1} = i\begin{pmatrix} -B & 0 \\ 0 & B \end{pmatrix}$$

$$-iv(t) \equiv T\begin{pmatrix} 0 & 0 \\ V & 0 \end{pmatrix}T^{-1} = \frac{i}{2}B^{-1/2}V(x, t)B^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}$$

If we define $\eta(t) = \langle \alpha(t), \beta(t) \rangle = T\langle w(t), w_t(t) \rangle$, then (279) becomes

$$\begin{aligned} \eta'(t) &= -ih_0\eta(t) - iv(t)\eta(t) \\ \eta(0) &= \langle \alpha_0(x), \beta_0(x) \rangle \equiv T\langle w(0), w_t(0) \rangle \end{aligned} \qquad (280)$$

for the $(\mathscr{h} \oplus \mathscr{h})$-valued function $\eta(t)$. h_0 is self-adjoint on $D(h_0) = D(B) \oplus D(B)$ and $v(t)$ is a continuous function from $\mathbb{R}$ into the bounded operators on $\mathscr{h} \oplus \mathscr{h}$ satisfying

$$\|v(t)\|_{\mathscr{L}(\mathscr{h} \oplus \mathscr{h})} \leq 2m^{-1} \sup_{x,t} |V(x, t)| \equiv M < \infty$$

Thus, for each t,

$$ih(t) \equiv i(h_0 + v(t))$$

is the generator of an exponentially bounded semigroup on $\mathscr{h} \oplus \mathscr{h}$, and all the $ih(t)$ have $D(h_0)$ as common domain by Theorem X.50. Further, since we are assuming that $V(x, t)$ is continuously differentiable, it is easy to check (Problem 137) that the operators $ih(t) + M + 1$ satisfy hypotheses (a)–(c) of Theorem X.70. Thus, Theorem X.70 implies that there exists a continuous family $u(t, s)$ of bounded operators on $\mathscr{h} \oplus \mathscr{h}$ so that $u(t, s)\eta_0$ is differentiable for $\eta_0 \in D(h_0)$ and

$$\begin{aligned} \frac{d}{dt} u(t, s)\eta_0 &= -ih(t)u(t, s)\eta_0 \\ u(s, s)\eta_0 &= \eta_0 \end{aligned} \tag{281}$$

Further, because of the bound on $\|v(t)\|$, $u(t, s)$ satisfies $\|u(t, s)\eta_0\| \leq e^{M|t-s|}\|\eta_0\|$. Notice that since $-ih(t)$ also generates an exponentially bounded semigroup, $u(t, s)$ is defined for all t and s and satisfies $u(t_1, t_2)u(t_2, t_3) = u(t_1, t_3)$. Since the propagation backward in time satisfies the same estimate as above, we have

$$e^{-M|t-s|}\|\eta_0\| \leq \|u(t, s)\eta_0\| \leq e^{M|t-s|}\|\eta_0\| \tag{282}$$

for all t and s. We remark that since the perturbations are bounded, we could have used the Dyson series in the interaction picture to define the dynamics (see the discussion after Theorem X.69) instead of the more subtle Theorem X.70.

The family of operators $T^{-1}u(t, s)T$ has two other important properties. First, the propagation is causal. That is, if $w_0 = \langle w(x, s), w_t(x, s)\rangle$ has support in Σ, then $w(t) = T^{-1}u(t, s)Tw_0$ has support in $\{x \mid |x - y| \leq |t - s|$ for some $y \in \Sigma\}$. The idea of the proof is exactly as in Theorem X.77 except that the nonlinear term $-|u|^2u$ is replaced by $V(x, t)w$. Secondly, let λ denote the operator

$$\lambda = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

on $\mathfrak{h} \oplus \mathfrak{h}$. Then,

$$u(t, s)^* \lambda u(t, s) = \lambda = u(t, s) \lambda u(t, s)^* \tag{283a}$$

for all t and s.

Before proving (283a), we note that, in terms of the original variables, it is equivalent to the statement that

$$q \equiv \int_{\mathbb{R}^3} [\overline{w(x, t)} w_t(x, t) - w(x, t) \overline{w_t(x, t)}] \, d^3x \tag{283b}$$

is independent of time for solutions w of (279). After we quantize, (283a) will express the conservation of "charge." To prove (283a) we note that by the boundedness of $u(t, s)$ and polarization, we need just show that

$$(u(t, s)\eta_0, \lambda u(t, s)\eta_0) = (\eta_0, \lambda \eta_0) = (u(t, s)^* \eta_0, \lambda u(t, s)^* \eta_0)$$

for η_0 in a dense set. It thus suffices to show that (283b) is time independent for solutions of (279) with initial data in $C_0^\infty(\mathbb{R}^3)$. The solution is then in $C_0^\infty(\mathbb{R}^3)$ for all times. Moreover, (283b) is just the Wronskian of the two solutions w and $\bar{w}$ of (279) and so is independent of time because the necessary integration by parts is permissible since $w(\cdot, t) \in C_0^\infty(\mathbb{R}^3)$. In terms of Noether's theorem, described in the appendix to Section 13, the conservation of q is an expression of the invariance $w \mapsto e^{i\theta} w$ (Problem 152).

We summarize:

Theorem XI.104 Let $V(x, t)$ be a continuously differentiable function of compact support in $\mathbb{R}^4$. Let $\mathfrak{h} \oplus \mathfrak{h}$, h_0 and $v(t)$ be as defined above. Then there exists a strongly continuous two-parameter family $u(t, s)$ of bounded operators on $\mathfrak{h} \oplus \mathfrak{h}$ such that:

(a) $u(t_3, t_2)u(t_2, t_1) = u(t_3, t_1)$; $u(t, t) = I$.
(b) If $\eta_0 \in D(h_0)$, then (281) holds and $\eta(t) = u(t, 0)\eta(0)$ satisfies (280).
(c) If supp $w(0) \in \Sigma$, then supp $T^{-1}u(t, 0)Tw(0) \subset \{x \,|\, |x - y| \le |t - s|$ for some $y \in \Sigma\}$.
(d) (283a) holds.
(e) Let $w_1 \in D(B^2)$ and $w_2 \in D(B)$ and set $\langle \alpha, \beta \rangle = T\langle w_1, w_2 \rangle$. Define $\langle \alpha(t), \beta(t) \rangle \equiv u(t, 0)\langle \alpha, \beta \rangle$. Then $w(t) = 2^{-1/2}\{B^{-1/2}\alpha(t) + B^{-1/2}\beta(t)\}$ is twice differentiable as an $L^2(\mathbb{R}^3)$-valued function and satisfies (279) with initial data $w(0) = w_1$, $w_t(0) = w_2$.

We have already proven (a)–(d). (e) holds because (279) and (280) are equivalent; one need only check the domain details (Problem 138).

We now introduce a classical interaction picture which will later be useful in the field theory situation. Let

$$\tilde{u}(t, s) = e^{ith_0}u(t, s)e^{-ish_0}$$

Then, for $\eta_0 \in D(h_0)$,

$$\begin{aligned}\frac{d}{dt}\tilde{u}(t, s)\eta_0 &= e^{ith_0}(-iv(t))u(t, s)e^{-ish_0}\eta_0\\ &= e^{+ith_0}(-iv(t))e^{-ith_0}(e^{+ith_0}u(t, s)e^{-ish_0})\eta_0\end{aligned}$$

so $\tilde{u}(t, s)\eta_0$ satisfies

$$\frac{d}{dt}\tilde{u}(t, s)\eta_0 = -i\tilde{v}(t)\tilde{u}(t, s)\eta_0$$

$$\tilde{u}(s, s)\eta_0 = \eta_0$$

where

$$\tilde{v}(t) = e^{+ith_0}v(t)e^{-ith_0}$$

Notice that by (282) and $u(s, t)u(t, s) = u(s, s) = I$, both $u(t, s)$ and $\tilde{u}(t, s)$ are bounded operators with bounded inverses.

We turn next to the classical scattering theory for (280) which is very easy because of our strong assumptions on $V(x, t)$. Let $u_0(t)$ denote e^{-ith_0} and let t_0 be large enough so that $v(x, t) = 0$ for $|t| \geq t_0$. Let $\eta_- \in \mathscr{h} \oplus \mathscr{h}$ be given and define $W_+ \eta_-$ to be that vector in $\mathscr{h} \oplus \mathscr{h}$ so that

$$\|u_0(t)\eta_- - u(t, 0)(W_+ \eta_-)\|_{\mathscr{h}\oplus\mathscr{h}} \to 0 \qquad \text{as} \quad t \to -\infty \tag{284}$$

By part (a) of Theorem XI.104,

$$\eta(x, t) \equiv u(t, -t_0)u_0(-t_0)\eta_-(x) = u(t, 0)u(0, -t_0)u_0(-t_0)\eta_-(x)$$

Moreover, for $t < -t_0$, $u(t, -t_0) = u_0(t + t_0)$ since $v(t) = 0$ for $t < -t_0$. Thus, for $t < -t_0$,

$$\eta(x, t) = u_0(t + t_0)u_0(-t_0)\eta_-(x) = u_0(t)\eta_-(x)$$

so if we set

$$W_+ \eta_- = u(0, -t_0)u_0(-t_0)\eta_-$$

then (284) holds since the norm is zero for $t < -t_0$. Similarly,

$$W_- \eta_+ = u(0, t_0)u_0(t_0)\eta_+$$

Since both u_0 and u are surjective, Ran $W_+ = \mathscr{h} \oplus \mathscr{h} =$ Ran W_-, so we have asymptotic completeness and

$$\begin{aligned} S_{\text{cl}} = W_-^{-1} W_+ &= [u(0, t_0)u_0(t_0)]^{-1}[u(0, -t_0)u_0(-t_0)] \\ &= u_0(-t_0)u(t_0, 0)u(0, -t_0)u_0(-t_0) \\ &= u_0(-t_0)u(t_0, -t_0)u_0(-t_0) \\ &= \tilde{u}(t_0, -t_0) \end{aligned}$$

Thus the classical scattering operator is just the interaction picture propagator from $-t_0$ to t_0.

We turn now to the field theory problem and begin by introducing the charged free scalar field of mass m. Let $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ be the boson Fock space over $L^2(\mathbb{R}^3)$ and let $a^\dagger(\cdot)$ and $a(\cdot)$ be the creation and annihilation operators on $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ occurring in (X.74), (X.75), and (X.76). As, in Section X.7, we denote by F_0 the finite particle vectors and set

$$D_{\mathscr{S}} = \{\psi \in F_0 \mid \psi^{(n)} \in \mathscr{S}(\mathbb{R}^{3n}) \quad \text{for all } n \geq 1\}$$

Let $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ be another copy of the same Fock space on which we denote the corresponding annihilation and creation operators by $b(\cdot)$ and $b^\dagger(\cdot)$. If $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ is the Hilbert space for some boson and $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ is the Hilbert space of the corresponding antiparticles, then the Hilbert space of the combined system is

$$\mathscr{H} \equiv \mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3)) = \mathscr{F}_s(\mathscr{h} \oplus \mathscr{h})$$

For each $f \in \mathscr{h}$, $a(f)$, $a^\dagger(f)$, $b(f)$, $b^\dagger(f)$ can be naturally identified with operators $a(f) \otimes I$, $a^\dagger(f) \otimes I$, $I \otimes b(f)$, $I \otimes b^\dagger(f)$ on $\mathscr{H}$ which we shall denote simply by $a(f)$, $a^\dagger(f)$, $b(f)$, and $b^\dagger(f)$ also. As described in Section X.7, one defines operator-valued distributions $a(p)$, $a^\dagger(p)$, $b(p)$, $b^\dagger(p)$. In terms of these annihilation and creation operators on $\mathscr{H}$ we define the **free Hamiltonian**

$$H_0 \equiv \int_{\mathbb{R}^3} \mu(p) a^\dagger(p) a(p)\, d^3p + \int_{\mathbb{R}^3} \mu(p) b^\dagger(p) b(p)\, d^3p$$

where $\mu(p) = \sqrt{p^2 + m^2}$, the **number operators**

$$N_+ \equiv \int_{\mathbb{R}^3} a^\dagger(p) a(p)\, d^3p$$

$$N_- \equiv \int_{\mathbb{R}^3} b^\dagger(p) b(p)\, d^3p$$

and the **charge operator**,

$$Q \equiv N_+ - N_-$$

Using Nelson's analytic vector theorem, it is easy to check that H_0, N_+, N_-, and Q are essentially self-adjoint on $D_{\mathscr{S}} \otimes D_{\mathscr{S}}$ which we shall denote simply by $D_{\mathscr{S}}$ from now on. We define the **charged free scalar Boson field** as the operator-valued distribution (note that the subscript zero refers to "free" and not to "time zero"):

$$\varphi_0(f, t) = \frac{1}{\sqrt{2}}\{a(e^{-iBt}B^{-1/2}f) + b^\dagger(e^{iBt}B^{-1/2}f)\}$$

for $f \in \mathscr{h}$. Formally, $\varphi_0(x, t)$ is just given by

$$\varphi_0(x, t) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} [e^{-i(\mu(p)t - p \cdot x)}a(p) + e^{i(\mu(p)t - p \cdot x)}b^\dagger(p)] \frac{d^3p}{\sqrt{2\mu(p)}}$$

We also define the **time-zero fields** by

$$\varphi_0(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{ip \cdot x}a(p) + e^{-ip \cdot x}b^\dagger(p)) \frac{d^3p}{\sqrt{2\mu(p)}}$$

$$\pi_0(x) \equiv \varphi_0(x)^* = \frac{i}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (e^{-ip \cdot x}a^\dagger(p) - e^{ip \cdot x}b(p)) \sqrt{\frac{\mu(p)}{2}}\, d^3p$$

$\varphi_0(x, t)$ is given in terms of the time zero field $\varphi_0(x)$ by the formula

$$\varphi_0(f, t) = e^{iH_0t}\varphi_0(f)e^{-iH_0t}$$

The creation and annihilation operators satisfy the commutation relations

$$[a(f), a^\dagger(g)] = (f, g)_{L^2}$$

$$[b(f), b^\dagger(g)] = (f, g)_{L^2}$$

$$[a^\#(f), b^\#(g)] = 0$$

for real-valued $f, g \in L^2(\mathbb{R}^3)$ where # denotes either a dagger or not.

If $\mathscr{U}^{(1)}$ and $\mathscr{U}^{(2)}$ are the actions of the Lorentz group on $\mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3))$ and $\mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$, we take $\mathscr{U} = \mathscr{U}^{(1)} \otimes \mathscr{U}^{(2)}$ to be the representation here. Finally, notice that we have a vacuum $\psi_0 = \psi_0^{(1)} \otimes \psi_0^{(2)}$ defined in terms of the vacua $\psi_0^{(i)}$ in $\mathscr{F}_s^{(i)}(L^2(\mathbb{R}^3))$. The quadruple $\langle \mathscr{H}, \mathscr{U}, \varphi_0(x, t), F_0 \rangle$ satisfies the obvious extension of the Gårding–Wightman axioms to non-Hermitian fields. This fact and the others claimed above may be verified just as in the case of the Hermitian scalar field discussed in Section X.7 (Problem 139).

Our problem is to solve the operator-valued Cauchy problem, that is, to find an operator-valued distribution $\varphi(x, t)$ that satisfies

$$\begin{gathered}\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t) \\ \varphi(x, 0) = \varphi_0(x) \\ \frac{d}{dt}\varphi(x, 0) = \pi_0(x)^*\end{gathered} \tag{285}$$

We proceed analogously to the classical case and first solve

$$\begin{aligned}\frac{d}{dt}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} &= i\begin{pmatrix} -B & 0 \\ 0 & B\end{pmatrix}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} \\ &\qquad + \frac{i}{2}B^{-1/2}VB^{-1/2}\begin{pmatrix} 1 & 1 \\ -1 & -1\end{pmatrix}\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} \\ &= -i(h_0 + v(t))\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} \\ a(x, 0) = a(x), &\qquad b^\dagger(x, 0) = b^\dagger(x)\end{aligned} \tag{286}$$

where $a(x)$ is the inverse Fourier transform of $a(p)$ and where the equation is supposed to hold in the (operator-valued) distributional sense. Since the equation is *linear*, we can solve it using the classical solution. If

$$u(t, 0) = \begin{pmatrix} u_{11}(t) & u_{12}(t) \\ u_{21}(t) & u_{22}(t)\end{pmatrix}$$

with $u_{ij}(t)$: $\mathscr{h} \to \mathscr{h}$, then, at least formally,

$$\begin{pmatrix} a(x, t) \\ b^\dagger(x, t)\end{pmatrix} = \begin{pmatrix} u_{11}(t) & u_{12}(t) \\ u_{21}(t) & u_{22}(t)\end{pmatrix}\begin{pmatrix} a(x) \\ b^\dagger(x)\end{pmatrix}$$

Thus, for $f \in \mathscr{h}$, we define the operator-valued distributions $a(\cdot, t)$ and $b^\dagger(\cdot, t)$ by

$$\begin{aligned} a(f, t) &= a(u_{11}^{\mathrm{T}}(t)f) + b^\dagger(u_{12}^{\mathrm{T}}(t)f) \\ b^\dagger(f, t) &= a(u_{21}^{\mathrm{T}}(t)f) + b^\dagger(u_{22}^{\mathrm{T}}(t)f)\end{aligned}$$

where $u_{ij}^{\mathrm{T}}(t)$, the transpose of $u_{ij}(t)$ on $\mathscr{h}$, is related to $u_{ij}(t)^*$ by $u_{ij}^{\mathrm{T}}(t) = Cu_{ij}(t)^*C$. We caution the reader that throughout the transposes are on

$\mathscr{h} = L^2(\mathbb{R}^3)$ and are not taken with respect to the two-by-two matrix structure. Finally, we define $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ by

$$\begin{aligned}\varphi(f, t) &= \frac{1}{\sqrt{2}}\{a(B^{-1/2}f, t) + b^{\dagger}(B^{-1/2}f, t)\}\\ &= \frac{1}{\sqrt{2}}\{a((u_{11}^{\mathrm{T}}(t) + u_{21}^{\mathrm{T}}(t))B^{-1/2}f)\\ &\qquad + b^{\dagger}((u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{-1/2}f)\} \qquad (287a)\end{aligned}$$

$$\begin{aligned}\pi(\bar{f}, t)^* &= \frac{i}{\sqrt{2}}\{-a(B^{1/2}f, t) + b^{\dagger}(B^{1/2}f, t)\}\\ &= \frac{i}{\sqrt{2}}\{a((-u_{11}^{\mathrm{T}}(t) + u_{21}^{\mathrm{T}}(t))B^{1/2}f)\\ &\qquad + b^{\dagger}((-u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{1/2}f)\} \qquad (287b)\end{aligned}$$

$\pi(\cdot, t)$ is only defined for $f \in D(B^{1/2})$. Because of (281), we have the following relations:

$$\begin{aligned}u'_{11}(t) + u'_{21}(t) &= -iB(u_{11}(t) - u_{21}(t))\\ u'_{12}(t) + u'_{22}(t) &= iB(-u_{12}(t) + u_{22}(t))\\ u''_{11}(t) + u''_{21}(t) &= (-B^2 + B^{1/2}VB^{-1/2})(u_{11}(t) + u_{21}(t))\\ u''_{12}(t) + u''_{22}(t) &= (-B^2 + B^{1/2}VB^{-1/2})(u_{12}(t) + u_{22}(t))\end{aligned}$$

Thus for $f \in D(B)$ real-valued,

$$\begin{aligned}\frac{d}{dt}\varphi(f, t) &= \frac{i}{\sqrt{2}}\{a([-B(u_{11}(t) - u_{21}(t)]^{\mathrm{T}}B^{-1/2}f)\\ &\qquad + b^{\dagger}([B(-u_{12}(t) + u_{22}(t))]^{\mathrm{T}}B^{-1/2}f)\}\\ &= \frac{i}{\sqrt{2}}\{-a((u_{11}^{\mathrm{T}}(t) - u_{21}^{\mathrm{T}}(t))B^{1/2}f)\\ &\qquad + b^{\dagger}((-u_{12}^{\mathrm{T}}(t) + u_{22}^{\mathrm{T}}(t))B^{1/2}f)\}\\ &= \pi(f, t)^*\end{aligned}$$

and, similarly, for $f \in D(B^2)$,

$$\frac{d^2}{dt^2}\varphi(f, t) = \varphi(-B^2 f, t) + \varphi(Vf, t)$$

which shows that $\varphi(\cdot, t)$ satisfies (285) in the sense of distributions.

In terms of the operators $a(f, t)$, $b^\dagger(f, t)$, we define in the natural way

$$a^\dagger(f, t) = a(Cf, t)^*$$
$$b(f, t) = b^\dagger(Cf, t)^*$$

Then at time t these operators satisfy the canonical commutation relations:

$$[a(f, t), a^\dagger(g, t)] = (Cf, g)$$
$$[b(f, t), b^\dagger(g, t)] = (Cf, g)$$
$$[a^\#(f, t), b^\#(g, t)] = 0$$

To see why this is true, note that

$$\begin{aligned} a(f, t) &= a(u^{\mathrm{T}}_{11} f) + b^\dagger(u^{\mathrm{T}}_{12} f) \\ a^\dagger(g, t) &= a(u^{\mathrm{T}}_{11} Cg)^* + b^\dagger(u^{\mathrm{T}}_{12} Cg)^* \\ &= a^\dagger(Cu^{\mathrm{T}}_{11} Cg) + b(Cu^{\mathrm{T}}_{12} Cg) \\ &= a^\dagger(u^*_{11} g) + b(u^*_{12} g) \end{aligned}$$

Thus

$$\begin{aligned} [a(f, t), a^\dagger(g, t)] &= [a(u^{\mathrm{T}}_{11} f), a^\dagger(u^*_{11} g)] + [b^\dagger(u^{\mathrm{T}}_{12} f), b(u^*_{12} g)] \\ &= (Cu^{\mathrm{T}}_{11} f, u^*_{11} g) - (Cu^*_{12} g, u^{\mathrm{T}}_{12} f) \\ &= (u^*_{11} Cf, u^*_{11} g) - (u^*_{12} Cf, u^*_{12} g) \\ &= (Cf, (u_{11} u^*_{11} - u_{12} u^*_{12}) g) \\ &= (Cf, g) \end{aligned}$$

since $u_{11} u^*_{11} - u_{12} u^*_{12} = I$ by (283a). The other commutators are computed similarly. It follows that

$$[\varphi(f, t), \pi(g, t)] = i(Cf, g)$$

Finally, we check that the field $\varphi(x, t)$ is causal, that is, that

$$[\varphi(f, t), \varphi(g, t')] = 0 \tag{288a}$$
$$[\varphi(f, t), \varphi(g, t')^*] = 0 \tag{288b}$$

if the sets $\{\langle x, t \rangle \mid x \in \operatorname{supp} f\}$ and $\{\langle x, t' \rangle \mid x \in \operatorname{supp} g\}$ are spacelike separated. Since $a(f)$ commutes with $a(g)$ for all f and g and similarly for $b(\cdot)$, (288a) holds automatically. We shall prove (288b) in the case where

$t' = 0$. The general case is proven similarly using the relation $u(t_1, t_2)u(t_2, t_3) = u(t_1, t_3)$ (Problem 140).

$$\begin{aligned}
[\varphi(f, t), \varphi(g)^*] &= \tfrac{1}{2}[a((u_{11} + u_{21})^{\mathrm{T}}B^{-1/2}f), a^\dagger(CB^{-1/2}g)] \\
&\quad + \tfrac{1}{2}[b^\dagger((u_{12} + u_{22})^{\mathrm{T}}B^{-1/2}f, b(CB^{-1/2}g)] \\
&= \tfrac{1}{2}(C(u_{11} + u_{21})^{\mathrm{T}}B^{-1/2}f, CB^{-1/2}g) \\
&\quad - \tfrac{1}{2}(B^{-1/2}g, (u_{21} + u_{22})^{\mathrm{T}}B^{-1/2}f) \\
&= \tfrac{1}{2}((u_{11} + u_{21})^*CB^{-1/2}f, CB^{-1/2}g) \\
&\quad - \tfrac{1}{2}((u_{21} + u_{22})^*CB^{-1/2}f, CB^{-1/2}g) \\
&= \tfrac{1}{2}(Cf, B^{-1/2}\{(u_{11} + u_{21}) - (u_{12} + u_{22})\}B^{-1/2}Cg)
\end{aligned}$$

Now let

$$d(t) = \begin{pmatrix} d_{11}(t) & d_{12}(t) \\ d_{21}(t) & d_{22}(t) \end{pmatrix} \equiv T^{-1}u(t, 0)T$$

Then $d_{12}(t) = B^{-1/2}\{(u_{11} + u_{21}) - (u_{12} + u_{22})\}B^{-1/2}$. Since the solution of the classical equation is causal, Theorem XI.104c, we conclude that $(Cf, d_{12}(t)Cg)$ is zero for $t < T$ if the supports of f and g are separated by a distance T.

We summarize:

Theorem XI.105 Let $\varphi(f, t)$ and $\pi(f, t)$ be given by (287). Then $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ are operator-valued distributions and

(a) $\varphi(\cdot, t)$ satisfies (285) where $\varphi_0(x)$ and $\pi_0(x)$ are the free time zero fields.

(b) $\dfrac{d}{dt}\varphi(\cdot, t) = \pi(\cdot, t)^*$.

(c) At each time t, $\varphi(\cdot, t)$ and $\pi(\cdot, t)$ satisfy the canonical commutation relations $[\varphi(f, t), \pi(g, t)] = i(Cf, g)$.

(d) Microscopic causality holds.

We turn now to the problem of scattering in the external field $V(x, t)$. Let $\varphi_{\text{in}}(x, t)$ denote the free charged scalar field of mass m with associated annihilation and creation operators a_{in} and $a_{\text{in}}^\dagger$. As before $V(x, t)$ is a real-valued function that is zero for $|t| \geq t_0$. We would like to solve the initial value problem

$$\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = V(x, t)\varphi(x, t) \tag{289}$$

$$\varphi(x, -t_0) = \varphi_{\text{in}}(x, -t_0)$$

$$\dot{\varphi}^*(x, -t_0) = \pi_{\text{in}}(x, -t_0)$$

If we define

$$a_{\text{in}}(f, t) \equiv e^{iH_0t}a_{\text{in}}(f)e^{-iH_0t} = a_{\text{in}}(e^{-iBt}f)$$

$$b^\dagger_{\text{in}}(f, t) \equiv e^{iH_0t}b^\dagger_{\text{in}}(f)e^{-iH_0t} = b^\dagger_{\text{in}}(e^{iBt}f)$$

Then $\varphi_{\text{in}}(x, -t_0)$ and $\pi_{\text{in}}(x, -t_0)$ are given in terms of $a_{\text{in}}(x)$ and $b^\dagger_{\text{in}}(x)$ by the formulas

$$\begin{aligned}\varphi_{\text{in}}(f, -t_0) &= \frac{1}{\sqrt{2}}\{a_{\text{in}}(B^{-1/2}f, -t_0) + b^\dagger_{\text{in}}(B^{-1/2}f, -t_0)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\text{in}}(e^{iBt_0}B^{-1/2}f) + b^\dagger_{\text{in}}(e^{-iBt_0}B^{-1/2}f)\}\end{aligned}$$

and

$$\pi_{\text{in}}(\bar{f}, -t_0)^* = \frac{i}{\sqrt{2}}\{-a_{\text{in}}(e^{iBt_0}B^{1/2}f) + b^\dagger_{\text{in}}(e^{-iBt_0}B^{1/2}f)\}$$

We can solve the initial value problem (289) analogously to the way we solved the initial value problem at $t = 0$. Set $u(t) = u(t, -t_0)$ and define

$$a(x, t) \equiv u_{11}(t)a_{\text{in}}(x, -t_0) + u_{12}(t)b^\dagger_{\text{in}}(x, -t_0)$$

$$b^\dagger(x, t) \equiv u_{21}(t)a_{\text{in}}(x, -t_0) + u_{22}(t)b^\dagger_{\text{in}}(x, -t_0)$$

and

$$\begin{aligned}\varphi(f, t) &\equiv \frac{1}{\sqrt{2}}\{a(B^{-1/2}f, t) + b^\dagger(B^{-1/2}f, t)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\text{in}}((u^{\mathrm{T}}_{11} + u^{\mathrm{T}}_{21})B^{-1/2}f, -t_0) \\ &\qquad + b^\dagger_{\text{in}}((u^{\mathrm{T}}_{12} + u^{\mathrm{T}}_{22})B^{-1/2}f, -t_0)\} \\ &= \frac{1}{\sqrt{2}}\{a_{\text{in}}(e^{iBt_0}(u^{\mathrm{T}}_{11} + u^{\mathrm{T}}_{21})B^{-1/2}f) \\ &\qquad + b^\dagger_{\text{in}}(e^{-iBt_0}(u^{\mathrm{T}}_{12} + u^{\mathrm{T}}_{22})B^{-1/2}f)\}\end{aligned}$$

$$\begin{aligned}\pi(f, t)^* &\equiv \frac{i}{\sqrt{2}}\{a_{\text{in}}(e^{iBt_0}(-u^{\mathrm{T}}_{11} + u^{\mathrm{T}}_{21})B^{1/2}f) \\ &\qquad + b^\dagger_{\text{in}}(e^{-iBt_0}(-u^{\mathrm{T}}_{12} + u^{\mathrm{T}}_{22})B^{1/2}f)\}\end{aligned}$$

Then, as above $d\varphi(f, t)/dt = \pi(f, t)$ and $\varphi(x, t)$ satisfies (289) in the sense of distributions. In fact, $\varphi(x, t) = \varphi_{\text{in}}(x, t)$ for all $t \le -t_0$.

Since $\varphi(x, t)$ satisfies (289) and $V(x, t) = 0$ for $t \ge t_0$, we have

$$\frac{d^2}{dt^2}\varphi(x, t) - \Delta\varphi(x, t) + m^2\varphi(x, t) = 0, \qquad t \ge t_0$$

That is, $\varphi(x, t)$ satisfies the free field equation for $t \ge t_0$. This suggests that we define

$$\begin{aligned} a_{\text{out}}(x, t_0) &= u_{11}(t_0, -t_0)a_{\text{in}}(x, -t_0) + u_{12}(t_0, -t_0)b_{\text{in}}^{\dagger}(x, -t_0) \\ b_{\text{out}}^{\dagger}(x, t_0) &= u_{22}(t_0, -t_0)a_{\text{in}}(x, -t_0) + u_{22}(t_0, -t_0)b_{\text{in}}^{\dagger}(x, -t_0) \end{aligned}$$

and

$$\begin{aligned} \varphi_{\text{out}}(f, t) &= \frac{1}{\sqrt{2}}\{a_{\text{out}}(e^{-i(t-t_0)B}B^{-1/2}f, t_0) \\ &\quad + b_{\text{out}}^{\dagger}(e^{i(t-t_0)B}B^{-1/2}f, t_0)\} \\ \pi_{\text{out}}(f, t)^* &= \frac{i}{\sqrt{2}}\{-a_{\text{out}}(e^{-i(t-t_0)B}B^{1/2}f, t_0) \\ &\quad + b_{\text{out}}^{\dagger}(e^{i(t-t_0)B}B^{1/2}f, t_0)\} \end{aligned}$$

For $f \in \mathscr{S}$, $a_{\text{out}}(f, t)$, $b_{\text{out}}^{\dagger}(f, t)$, $\varphi_{\text{out}}(f, t)$, and $\pi_{\text{out}}(f, t)$ and all their products are well-defined operators on $D_{\mathscr{S}}$. Further, $d\varphi_{\text{out}}(f, t)/dt = \pi_{\text{out}}(f, t)$ and $\varphi_{\text{out}}(x, t)$ is a "free field" in the sense that it satisfies the free Klein–Gordon equation for all t. Notice also that $\varphi(x, t) = \varphi_{\text{out}}(x, t)$ for all $t \ge t_0$. We shall see later, though it is not obvious a priori, that there is a vacuum ψ_{out} for the out fields, that

$$H_{\text{out}} = \int_{\mathbb{R}^3} \mu(p)a_{\text{out}}^{\dagger}(p, t_0)a_{\text{out}}(p, t_0)\, d^3p + \int_{\mathbb{R}^3} \mu(p)b_{\text{out}}^{\dagger}(p, t_0)b_{\text{out}}(p, t_0)\, d^3p \tag{290}$$

makes sense as a self-adjoint operator on $\mathscr{H}$ and that

$$\begin{aligned} \varphi_{\text{out}}(x, t) &= e^{iH_{\text{out}}(t-t_0)}\varphi_{\text{out}}(x, t_0)e^{-iH_{\text{out}}(t-t_0)} \\ \pi_{\text{out}}(x, t) &= e^{iH_{\text{out}}(t-t_0)}\pi_{\text{out}}(x, t_0)e^{-iH_{\text{out}}(t, -t_0)} \end{aligned}$$

Since a_{out} has some $b_{\text{in}}^{\dagger}$ in it, H_{out} will not annihilate ψ_{in}, so $H_{\text{out}} \ne H_{\text{in}} \equiv H_0$. Thus, the asymptotic free dynamics near $t = +\infty$ is not the same as the asymptotic free dynamics near $t = -\infty$. The dynamical situation is described by Fig. XI.15. In accordance with the general ideas of this chapter we should define a scattering transformation $\mathfrak{S}$ as a map from

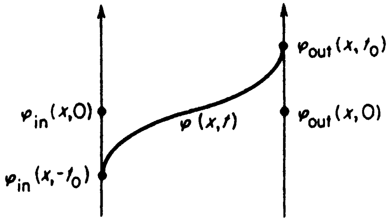


FIGURE XI.15

operators to operators given by

$$\mathfrak{S}\colon \varphi_{\text{in}}(x, 0) \to \varphi_{\text{out}}(x, 0)$$
$$\mathfrak{S}\colon \pi_{\text{in}}(x, 0) \to \pi_{\text{out}}(x, 0)$$

We shall see that $\mathfrak{S}$ is unitarily implementable, that is, that there exists a unitary operator S on $\mathscr{H}$ such that

$$\varphi_{\text{out}}(f, 0) = S^{-1}\varphi_{\text{in}}(f, 0)S$$
$$\pi_{\text{out}}(f, 0) = S^{-1}\pi_{\text{in}}(f, 0)S$$

We shall call S the **scattering operator** and $\mathfrak{S}$ the **Heisenberg picture scattering operator** since $\mathfrak{S}$ represents the scattering transformation in the Heisenberg picture of quantum mechanics. Notice that S can only be determined up to a phase by these conditions. The convention on S corresponds to using the Jauch S-matrix as opposed to the EBFM S-matrix which we have used thus far in this volume. This choice is universal in field theory and we will use it again in the next section. We have the following explicit action of $\mathfrak{S}$:

$$\begin{aligned}
\mathfrak{S}(a_{\text{in}}(f)) &= a_{\text{out}}(f, 0) \\
&= \frac{1}{\sqrt{2}}\{\varphi_{\text{out}}(f, 0) + i\pi(f, 0)^*\} \\
&= a_{\text{out}}(e^{it_0B}f, t_0) \\
&= a_{\text{in}}(u_{11}^{\text{T}}(t_0, -t_0)e^{it_0B}f, -t_0) \\
&\quad + b_{\text{in}}^{\dagger}(u_{12}^{\text{T}}(t_0, -t_0)e^{it_0B}f, -t_0) \\
&= a_{\text{in}}(e^{it_0B}u_{11}^{\text{T}}(t_0, -t_0)e^{it_0B}f) \\
&\quad + b_{\text{in}}^{\dagger}(e^{-it_0B}u_{12}^{\text{T}}(t_0, -t_0)e^{it_0B}f) \\
&= a_{\text{in}}(\tilde{u}_{11}^{\text{T}}(t_0, -t_0)f) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\text{T}}(t_0, -t_0)f)
\end{aligned}$$

and similarly

$$\begin{aligned}
\mathfrak{S}(b_{\text{in}}^{\dagger}(f)) &= b_{\text{out}}^{\dagger}(f, 0) \\
&= a_{\text{in}}(\tilde{u}_{21}^{\text{T}}(t_0, -t_0)f) + b_{\text{in}}^{\dagger}(\tilde{u}_{22}^{\text{T}}(t_0, -t_0)f)
\end{aligned}$$

Thus the transformation from time zero annihilation and creation operators of the in field to the time zero annihilation and creation operators of the out field is given by

$$\begin{pmatrix} a_{\text{out}}(x, 0) \\ b_{\text{out}}^{\dagger}(x, 0) \end{pmatrix} = S_{\text{cl}} \begin{pmatrix} a_{\text{in}}(x) \\ b_{\text{in}}^{\dagger}(x) \end{pmatrix}$$

where

$$S_{\text{cl}} = \tilde{u}(t_0, -t_0) = e^{it_0h_0}u(t_0, -t_0)e^{it_0h_0}$$

is the classical scattering operator.

We seek to construct a unitary S so that

$$S^{-1}a_{\text{in}}^{*}(f)S = a_{\text{out}}^{*}(f)$$

$$S^{-1}b_{\text{in}}^{*}(f)S = b_{\text{out}}^{*}(f) \tag{291}$$

where $a_{\text{out}}^{\dagger}$, b_{out} are given in terms of a_{out}, $b_{\text{out}}^{\dagger}$ by the usual formulas involving the conjugation C. Since h_0 commutes with λ and (283) holds, $\tilde{u}(t_0, -t_0)$ satisfies

$$\tilde{u}(t_0, -t_0)^{*}\lambda\tilde{u}(t_0, -t_0) = \lambda = \tilde{u}(t_0, -t_0)\lambda\tilde{u}(t_0, -t_0)^{*} \tag{292}$$

Thus, the same proof as in Theorem XI.105 shows that a_{out}, b_{out} satisfy the canonical commutation relations

$$[a_{\text{out}}(f, 0), a_{\text{out}}^{\dagger}(g, 0)] = (Cf, g)$$

$$[b_{\text{out}}(f, 0), b_{\text{out}}^{\dagger}(g, 0)] = (Cf, g)$$

and that all other commutators vanish.

The following theorem reduces the question of unitary implementability to a property of the classical propagation.

Theorem XI.106 Suppose that $\tilde{u}_{11}(t_0, -t_0)^{-1}\tilde{u}_{12}(t_0, -t_0)$ is a Hilbert–Schmidt operator on $L^2(\mathbb{R}^3)$. Then there is a unitary operator S on $\mathscr{H} = \mathscr{F}_s^{(1)}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}_s^{(2)}(L^2(\mathbb{R}^3))$ so that (291) holds.

Proof Since $\tilde{u}$ satisfies (292), we have that

$$\tilde{u}_{11}^{*}\tilde{u}_{11} = 1 + \tilde{u}_{12}^{*}\tilde{u}_{12}, \qquad \tilde{u}_{11}\tilde{u}_{11}^{*} = 1 + \tilde{u}_{12}\tilde{u}_{12}^{*} \tag{293}$$

so $\tilde{u}_{11}^{*}\tilde{u}_{11} \geq 1$ and $\tilde{u}_{11}\tilde{u}_{11}^{*} \geq 1$, from which it follows that $\operatorname{Ran} \tilde{u}_{11} = L^2(\mathbb{R}^3)$ and that $\tilde{u}_{11}^{-1}$ exists and is bounded. Thus, $\tilde{u}_{11}(t_0, -t_0)^{-1}\tilde{u}_{12}(t_0, -t_0)$ makes sense.

To prove the theorem we construct a vector ψ_{out} in $\mathscr{H}$ which is a vacuum for the out fields. Once this is done, it will be easy to write down S^{-1} explicitly.

According to Theorems VI.17 and VI.22e and the hypothesis, there exist orthonormal sets $\{f_i\}$, $\{g_i\}$ in $L^2(\mathbb{R}^3)$ so that $L = \tilde{u}_{11}^{-1}\tilde{u}_{12}$ may be written

$$Lh = \sum_{i=1}^{N_0} \lambda_i(g_i, h)f_i$$

where the λ_i are the eigenvalues of $|L|$ and $\sum \lambda_i^2 < \infty$. N_0 may be finite or infinite; we will consider the case $N_0 = \infty$ since that is where most of the difficulties occur. From (293) it follows that

$$1 = LL^* + (\tilde{u}_{11}^{-1})(\tilde{u}_{11}^{-1})^* \tag{294}$$

and since $LL^*h = \sum \lambda_i^2(f_i, h)f_i$, it follows that $\lambda_i \le 1$ since $(\tilde{u}_{11}^{-1})(\tilde{u}_{11}^{-1})^* \ge 0$. Furthermore, if $\lambda_{i_0} = 1$ for some i_0, (294) implies that $(\tilde{u}_{11}^{-1})^*f_i = 0$, which is impossible since Ran $\tilde{u}_{11}^{-1} = L^2(\mathbb{R}^3)$. Thus, $\lambda_i < 1$ for all i.

Now, denote the vacuum in $\mathscr{H}$ by ψ_{in} and let F_{in} be the set of finite linear combination of vectors of the form $\psi_1 \otimes \psi_2$ where $\psi_i \in F_0 \subset \mathscr{F}_s(L^2(\mathbb{R}^3))$. In terms of the orthonormal sets $\{f_i\}$, $\{g_i\}$, we define

$$a_i = a_{\text{in}}(Cf_i), \qquad b_i = b_{\text{in}}(g_i)$$

The out vacuum is given formally by

$$\psi_{\text{out}} = d\left(\prod_{i=1}^{\infty} e^{-\lambda_i a_i{}^* b_i{}^*}\right)\psi_{\text{in}}$$

where the constant d is chosen so that $\|\psi_{\text{out}}\| = 1$. To make sense out of this expression let us begin by looking at $e^{-\lambda_1 a_1{}^* b_1{}^*}\psi_{\text{in}}$ which we define by the power series

$$e^{-\lambda_1 a_1{}^* b_1{}^*}\psi_{\text{in}} = \sum_{n=0}^{\infty} \frac{(-\lambda_1 a_1^* b_1^*)^n}{n!}\psi_{\text{in}}$$

For each n, ψ_{in} is in the domain of $(a_1^* b_1^*)^n$ and

$$\begin{aligned}(a_1^* b_1^*)^n\psi_{\text{in}} &= \left[\sqrt{n!}\, S_n\left(\overset{n}{\otimes} f_1\right)\right] \otimes \left[\sqrt{n!}\, S_n\left(\overset{n}{\otimes} \bar{g}_1\right)\right] \\ &= n!\left(\overset{n}{\otimes} f_1\right) \otimes \left(\overset{n}{\otimes} \bar{g}_1\right)\end{aligned}$$

For different n, the vectors $(a_1^* b_1^*)^n\psi_{\text{in}}$ are orthogonal, so

$$\begin{aligned}\|e^{-\lambda_1 a_1{}^* b_1{}^*}\psi_{\text{in}}\|^2 &= \sum_{n=0}^{\infty} \frac{\lambda_1^{2n}}{(n!)^2}\|(a_1^* b_1^*)^n\psi_{\text{in}}\|^2 \\ &= \sum_{n=0}^{\infty} \lambda_1^{2n} = \frac{1}{1-\lambda_1^2}\end{aligned}$$

Thus $e^{-\lambda_1 a_1{}^* b_1{}^*}\psi_{\text{in}}$ makes sense since $\lambda_1 < 1$. Similarly, using the fact that $(f_1, f_2) = 0 = (g_1, g_2)$, we have

$$(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s \psi_{\text{in}} = \left[\sqrt{n!}\, S_n\left(\overset{n-s}{\otimes} f_2 \overset{s}{\otimes} f_1\right)\right] \otimes \left[\sqrt{n!}\, S_n\left(\overset{n-s}{\otimes} \bar{g}_2 \overset{s}{\otimes} \bar{g}_1\right)\right]$$

so

$$\|(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s \psi_{\text{in}}\|^2 = (n!)^2 \left[\frac{(n-s)!s!}{n!}\right]^2 = [(n-s)!s!]^2$$

Thus

$$\begin{aligned}
&\|e^{-\lambda_2 a_2{}^* b_2{}^*} e^{-\lambda_1 a_1{}^* b_1{}^*} \psi_{\text{in}}\|^2 \\
&\quad = \left\|\sum_{n=0}^{\infty} \frac{1}{n!}(-\lambda_1 a_1^* b_1^* - \lambda_2 a_2^* b_2^*)^n \psi_{\text{in}}\right\|^2 \\
&\quad = \sum_{n=0}^{\infty} \left(\frac{1}{n!}\right)^2 \sum_{s=0}^{n} \left(\frac{n!}{(n-s)!s!}\right)^2 \lambda_1^{2s} \lambda_2^{2(n-s)} \|(a_2^* b_2^*)^{n-s}(a_1^* b_1^*)^s \psi_{\text{in}}\|^2 \\
&\quad = \sum_{n=0}^{\infty} \sum_{s=0}^{n} \lambda_1^{2s} \lambda_2^{2(n-s)} \\
&\quad = \frac{1}{1-\lambda_1^2} \frac{1}{1-\lambda_2^2}
\end{aligned}$$

Continuing in this way, we show that

$$\chi_N = \left(\prod_{i=1}^{N} e^{-\lambda_i a_i{}^* b_i{}^*}\right) \psi_{\text{in}}$$

exists and that

$$\|\chi_N\|^2 = \prod_{i=1}^{N} \left(\frac{1}{1-\lambda_i^2}\right)$$

Furthermore, using the orthogonality of the $\{f_i\}$ among themselves and the $\{g_i\}$ among themselves, it follows similarly to the above calculation (Problem 141a) that

$$\|\chi_N - \chi_M\|^2 = \prod_{i=1}^{N} \left(\frac{1}{1-\lambda_i^2}\right) - \prod_{i=1}^{M} \left(\frac{1}{1-\lambda_i^2}\right) \tag{295}$$

Because of the Hilbert–Schmidt assumption, $\sum \lambda_i^2 < \infty$, so the infinite product $\prod_{i=1}^{\infty} (1 - \lambda_i^2)^{-1}$ converges. Thus, χ_N is Cauchy as $N \to \infty$ and we define the limit, suitably normalized, as ψ_{out}.

To prove that ψ_{out} is annihilated by $a_{\text{out}}(f)$ recall that

$$a_{\text{out}}(f) = a_{\text{in}}(\tilde{u}_{11}^{\mathrm{T}} f) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}} f)$$

Since $\operatorname{Ran}(\tilde{u}_{11}^{\mathrm{T}})^{-1} = L^2(\mathbb{R}^3)$, we may suppose that f is of the form $f = (\tilde{u}_{11}^{\mathrm{T}})^{-1} h$. Choose $h = Cf_i$. Then

$$\begin{aligned} a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} Cf_i) &= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}}(\tilde{u}_{11}^{\mathrm{T}})^{-1} Cf_i) \\ &= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(C((\tilde{u}_{11})^{-1}\tilde{u}_{12})^* f_i) \\ &= a_{\text{in}}(Cf_i) + b_{\text{in}}^{\dagger}(C\lambda_i g_i) \\ &= a_i + \lambda_i b_i^* \end{aligned}$$

By the orthogonality of the $\{f_i\}$ and $\{g_i\}$, the a_i^* and b_i^* all commute for different i, so

$$\begin{aligned} (a_i + \lambda_i b_i^*)\chi_N &= \left(\prod_{j \neq i}^{N} e^{-\lambda_j a_j^* b_j^*} \right) (a_i + \lambda_i b_i^*) e^{-\lambda_i a_i^* b_i^*} \psi_{\text{in}} \\ &= 0 \end{aligned}$$

since $(a_i + \lambda_i b_i^*) e^{-\lambda_i a_i^* b_i^*} \psi_{\text{in}} = 0$ on account of the canonical commutation relations satisfied by a_i and a_i^* (Problem 141b). Letting $N \to \infty$ we see that ψ_{out} is in the domain of $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} Cf_i)$ and that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} Cf_i)\psi_{\text{out}} = 0$. Suppose that $k \in \{f_i\}^{\perp}$. Then $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} Ck) = a_{\text{in}}(Ck)$ and since $a_{\text{in}}(Ck)$ commutes with a_i^* and b_i^* for all i, we conclude that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} Ck)\psi_{\text{out}} = 0$ also. Expanding an arbitrary $h \in L^2(\mathbb{R}^3)$ in terms of $\{f_i\}$ and a basis for $\{f_i\}^{\perp}$, one easily shows from this that ψ_{out} is in the domain of $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} h)$ and that $a_{\text{out}}((\tilde{u}_{11}^{\mathrm{T}})^{-1} h)\psi_{\text{out}} = 0$. The proof that b_{out} annihilates ψ_{out} is similar and uses $\tilde{u}_{21}^*(\tilde{u}_{22}^*)^{-1} = \tilde{u}_{11}^{-1}\tilde{u}_{12}$ which follows from the fact that $\tilde{u}$ satisfies (292).

Define

$$h_i = (\tilde{u}_{11}^{-1}) * f_i / \sqrt{1 - \lambda_i^2}, \qquad k_i = (\tilde{u}_{22}^{-1}) * g_i / \sqrt{1 - \lambda_i^2}$$

and

$$\tilde{a}_i \equiv a_{\text{out}}(Ch_i), \qquad \tilde{b}_i \equiv b_{\text{out}}(k_i)$$

Then, calculating as above,

$$\tilde{a}_i = a_{\text{in}}(\tilde{u}_{11}^{\mathrm{T}} Ch_i) + b_{\text{in}}^{\dagger}(\tilde{u}_{12}^{\mathrm{T}} Ch_i) = \frac{a_i + \lambda_i b_i^*}{\sqrt{1 - \lambda_i^2}}$$

and

$$\tilde{b}_i = \frac{b_i + \lambda_i a_i^*}{\sqrt{1 - \lambda_i^2}}$$

It follows easily from (294) that $\{h_i\}$ is an orthonormal set. To see that $\{k_i\}$ is an orthonormal set, one first uses (283a) to prove that

$$\begin{aligned}\sum_{i=1}^{\infty} \lambda_i^2 (g_i, \cdot\,) g_i &= LL^* \\ &= \tilde{u}_{22}^{-1} \tilde{u}_{21} \tilde{u}_{21}^* (\tilde{u}_{22}^{-1})^* \\ &= I - \tilde{u}_{22}^{-1} (\tilde{u}_{22}^{-1})^*\end{aligned}$$

from which the orthonormality follows easily. We now extend $\{h_i\}$ to an orthonormal basis for $L^2(\mathbb{R}^3)$ which we denote by $\{\eta_i\}$ and extend $\{Ck_i\}$ to an orthonormal basis which we denote by $\{\gamma_i\}$. For vectors of the form $\prod a_{\text{in}}^\dagger(\eta_i) \prod b_{\text{in}}^\dagger(\gamma_j)\psi_{\text{in}}$, we define S^{-1} by

$$S^{-1}: \psi_{\text{in}} \to \psi_{\text{out}}$$

$$S^{-1} \prod a_{\text{in}}^\dagger(\eta_i) \prod b_{\text{in}}^\dagger(\gamma_j)\psi_{\text{in}} \to \prod a_{\text{out}}^\dagger(\eta_i) \prod b_{\text{out}}^\dagger(\gamma_j)\psi_{\text{out}}$$

where the products are taken over some finite collections of i's and j's. First, notice that the right-hand side makes sense because ψ_{out} is in the domain of $\prod a_{\text{out}}^\dagger(\eta_i) \prod b_{\text{out}}^\dagger(\gamma_j)$. If $\eta_i = (\tilde{u}_{11}^{-1})^* f_i / \sqrt{1 - \lambda_i^2}$, then

$$a_{\text{out}}^\dagger(\eta_i) = (a_i^* + \lambda_i b_i)/\sqrt{1 - \lambda_i^2}.$$

On the other hand, if η_i is one of the other basis elements, then $\eta_i = (\tilde{u}_{11}^{-1})^* f$ where $f \in \{f_i\}^\perp$ and $\|f\| = 1$. This is because (294) implies that $(\tilde{u}_{11}^{-1})^*$ is an isometry from $\{f_i\}^\perp$ to $\{(\tilde{u}_{11}^{-1})^*[\{f_i\}]\}^\perp$. So, in this case $a_{\text{out}}^\dagger(\eta_i) = a_{\text{in}}(Cf)^*$ where $f \perp \{f_i\}$. Similar statements hold for the $a_{\text{out}}^\dagger(\gamma_i)$ based on properties of $(\tilde{u}_{22}^{-1})^*$. Thus each term in $\prod a_{\text{out}}^\dagger(\eta_i) \prod b_{\text{out}}^\dagger(\gamma_j)$ is a product of a finite number of powers of a_i^*, b_i^*, $a_{\text{in}}(Cf)$, $b_{\text{in}}(g)$. When such products are applied to χ_N the asserted limit (ψ_{out}) still exists since a_i^*, b_i^* do not affect χ_N for $N > i$ and $a_{\text{in}}(Cf)$, $b_{\text{in}}(g)$ commute with $e^{-\lambda_i a_i^* b_i^*}$ for all i and, when taken inside, do not affect the estimates because $f \perp \{f_i\}$, $g \perp \{g_i\}$. This same orthogonality and the definitions of $\tilde{a}_i$, $\tilde{b}_i$ ensure that $a_{\text{out}}^\dagger(\eta_i)$, $a_{\text{out}}(C\eta_i)$, $b_{\text{out}}^\dagger(\gamma_i)$, $b_{\text{out}}(C\gamma_i)$ satisfy the canonical commutation relations, from which it follows that S^{-1} is norm preserving and orthogonality preserving on the orthonormal basis $\{\prod a_{\text{in}}^\dagger(\eta_i) \prod b_{\text{in}}^\dagger(\gamma_i)\psi_{\text{in}}\}$ for $\mathscr{H}$. Thus S^{-1} extends uniquely to an isometry of $\mathscr{H}$ into $\mathscr{H}$, and it is easy to check that (291) holds. The reader is asked to fill in the details of the above argument in Problem 141c.

In order to show that S^{-1} is unitary we need just show that S^{-1} has a dense range and to do that it is sufficient to show that every vector of the form $\prod a_{\rm in}^\dagger(\eta_i) \prod b_{\rm in}^\dagger(\gamma_i)\psi_{\rm in}$ can be approximated by finite linear combinations of vectors of the form $\prod a_{\rm out}^\dagger(\eta_i) \prod b_{\rm out}^\dagger(\gamma_i)\psi_{\rm out}$. To see that this is so, define $\psi'_{\rm in} = d' \prod_{i=1}^{\infty} e^{\lambda_i \tilde{a}_i^* \tilde{b}_i^*}\psi_{\rm out}$. The same proofs as in the construction of $\psi_{\rm out}$ show that the right-hand side converges and that $a_{\rm in}(C\eta_i)\psi'_{\rm in} = 0 = b_{\rm in}(C\gamma_j)\psi'_{\rm in}$ for all i and j. Thus, adjusting the constant d', we have $\psi'_{\rm in} = \psi_{\rm in}$, and

$$\prod a_{\rm in}^\dagger(\eta_i) \prod b_{\rm in}^\dagger(\gamma_i)\psi_{\rm in} = \prod a_{\rm in}^\dagger(\eta_i) \prod b_{\rm in}^\dagger(\gamma_i)\, d' \prod_{n=1}^{\infty} e^{\lambda_n \tilde{a}_n^* \tilde{b}_n^*}\psi_{\rm out}.$$

Since $a_{\rm in}^\dagger(\eta_i)$ and $b_{\rm in}^\dagger(\gamma_i)$ can be expressed in terms of $\tilde{a}_i^*$, $\tilde{b}_i^*$, or directly in terms of $a_{\rm out}^\dagger$, $b_{\rm out}^\dagger$, and we can make the infinite product finite and terminate the remaining exponentials after finitely many terms, the left-hand side can be approximated by finite linear combinations of terms of the form $\prod a_{\rm out}^\dagger(\eta_i) \prod b_{\rm out}^\dagger(\gamma_j)\psi_{\rm out}$ as required. ∎

Before proving that $\tilde{u}_{12}(t_0, -t_0)$ is Hilbert–Schmidt, we make several remarks about the proof just completed. First, the argument can be turned around to show that if the map $a_{\rm in} \to a_{\rm out}$, $b_{\rm in} \to b_{\rm out}$ is unitarily implementable, then $\tilde{u}_{11}^{-1}\tilde{u}_{12}$ is Hilbert–Schmidt. Secondly, the proof depended only on the Hilbert–Schmidt hypothesis and (292) and so the same proof together with the proposition below shows that for each t, there is a unitary operator $U(t, -t_0)$ so that

$$\varphi(x, t) = U(t, -t_0)\varphi_{\rm in}(x, -t_0)U(t, -t_0)^{-1}$$

$$\pi(x, t) = U(t, -t_0)\pi_{\rm in}(x, -t_0)U(t, -t_0)^{-1}$$

that is, the dynamics given by Theorem XI.105 is unitarily implementable. Finally, if we set $H_{\rm out} = S^{-1}H_{\rm in}S$, then $H_{\rm out}$ is given by

$$H_{\rm out} = \int_{\mathbb{R}^3} \mu(p)a_{\rm out}^\dagger(p, 0)a_{\rm out}(p, 0)\, dp + \int_{\mathbb{R}^3} \mu(p)b_{\rm out}^\dagger(p, 0)b_{\rm out}(p, 0)\, dp$$

$H_{\rm out}$ is also given by (290), and the free dynamics of the out fields is given by $e^{itH_{\rm out}}$. All of these facts are trivial once one has S since they are just the translations of facts about the (free) in field.

Proposition Suppose that $V(x, t)$ is C^∞ with compact support in $\mathbb{R}^4$. Then the operators $u_{12}(t, -t_0)$ and $\tilde{u}_{12}(t, -t_0)$ described above are Hilbert–Schmidt on $L^2(\mathbb{R}^3)$.

Proof Since $u_{12}(t, s) = e^{-itB}\tilde{u}_{12}(t, s)e^{-isB}$, it suffices to prove that $\tilde{u}_{12}(t, -t_0)$ is Hilbert–Schmidt. Since $t \to \tilde{v}(t)$ is a strongly continuous map of $\mathbb{R}$ into the bounded operators on $L^2(\mathbb{R}^3)$, $\tilde{u}(t, -t_0)$ is given by the Dyson series (Theorem X.69):

$$\tilde{u}(t, -t_0)f = f + \sum_{n=1}^{\infty} (-i)^n \int_{-t_0}^{t} \int_{-t_0}^{t_1} \cdots \int_{-t_0}^{t_{n-1}} \tilde{v}(t_1) \cdots \tilde{v}(t_n) f \, dt_n \cdots dt_1 \tag{296}$$

The first try one might make for showing that $\tilde{u}_{12}$ is Hilbert–Schmidt is to prove that $M_2 \equiv \sup_t \|\tilde{v}(t)\|_{\mathscr{I}_2} < \infty$ for then the nth term in (296) would be Hilbert–Schmidt with Hilbert–Schmidt norm bounded by $|t_0 + t|^n M_2^n/n!$. Unfortunately, M_2 is infinite since

$$\tilde{v}(t) = \begin{pmatrix} e^{iBt}Re^{-iBt} & e^{+iBt}Re^{iBt} \\ -e^{-iBt}Re^{-iBt} & -e^{-iBt}Re^{iBt} \end{pmatrix}$$

where $R = -\frac{1}{2}B^{-1/2}V(x, t)B^{-1/2}$, so

$$\operatorname{Tr}(R^*R) = \tfrac{1}{4} \int |\hat{V}(k - p, t)|^2 (k^2 + m^2)^{-1/2} (p^2 + m^2)^{-1/2} \, d^3k \, d^3p$$

is infinite since the integrand falls only as $|k + p|^{-2}$ as $|k + p| \to \infty$ with $k - p$ fixed. However

$$M_4 \equiv \sup_t \|\tilde{v}(t)\|_{\mathscr{I}_4} < \infty$$

since $|V(x, t)|^{1/2}B^{-1/2}$ is in $\mathscr{I}_8$ by Theorem XI.20 and the fact that $f(y) = (y^2 + m^2)^{-1/4} \in L^8(\mathbb{R}^3)$. Since $\|AB\|_{\mathscr{I}_2} \le \|A\|_4 \|B\|_4$, the nth term on the right of (296) for $n \ge 2$ is Hilbert–Schmidt with Hilbert–Schmidt norm bounded by $M_4^n \, |t_0 + t|^n/n!$ Thus since the $n = 0$ term has no 12 element, it suffices to prove that

$$G(t) = \int_{-t_0}^{t} \tilde{v}_{12}(s) \, ds$$

is Hilbert–Schmidt (this would *not* be true if we replaced 12 by 11). Now, $G(t)$ has p-space integral kernel

$$g(k, p, t) = \int_{-t_0}^{t} (k^2 + m^2)^{-1/4} (p^2 + m^2)^{-1/4} \hat{V}(k - p, s) \times \exp[-is(\sqrt{k^2 + m^2} + \sqrt{p^2 + m^2})] \, ds$$

and an integration by parts easily shows that

$$|g(k, p, t)| \le C[(k^2 + m^2)^{-1/4}(p^2 + m^2)^{-1/4}\{(k^2 + m^2)^{1/2} + (p^2 + m^2)^{1/2}\}^{-1}(1 + |k - p|^2)^{-4}] \tag{297}$$

Thus $g \in L^2(\mathbb{R}^6)$ for each t so $G(t)$ is Hilbert–Schmidt. ▌

This calculation has an intriguing feature when done in four space dimensions. Then (297) is not in L^2, so it is natural to attempt to integrate by parts again. If there is no boundary term from the first integration by parts, then one can improve the falloff and thereby control the $n = 1$ term in (296); but if the boundary term is nonzero, the $n = 1$ term will *not* be Hilbert–Schmidt. For all t, the $n \ge 3$ terms are Hilbert–Schmidt by a direct argument since in this case $M_6 < \infty$, and the $n = 2$ term is Hilbert–Schmidt using a single integration by parts. Since $\hat{V}(\cdot, -t_0) = 0$, the boundary term is not in L^2 if $\hat{V}(\cdot, t) \ne 0$ and therefore we have that in the four space dimensional case, $u_{12}(t, -t_0)$ is Hilbert–Schmidt only for those t with $V(\cdot, t) = 0$. Thus, it can happen that the S-operator *is* unitarily implementable in cases where the dynamics is not implementable for intermediate times. This phenomenon also takes place in three space dimensions if one considers suitable higher spin equations or uses coupling different from that in (278).

We summarize:

Theorem XI.107 Assume that $V(x, t)$ is C^∞ with compact support in $\mathbb{R}^4$. Let φ_{in} be the free charged scalar field of mass m. Then there exist operator-valued distributions $\varphi(x, t)$, $\pi(x, t)$ for each t so that $\pi(x, t) = d\varphi(x, t)/dt$ and (289) holds. There exists a family of unitary operators $U(t, -t_0)$ on $\mathscr{H}$ so that

$$\varphi(x, t) = U(t, -t_0)\varphi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1}$$

$$\pi(x, t) = U(t, -t_0)\pi_{\text{in}}(x, -t_0)U(t, -t_0)^{-1}$$

Finally, let φ_{out} be as defined above. Then there exists a unitary scattering operator S on $\mathscr{H}$ so that

$$\varphi_{\text{out}}(x, 0) = S^{-1}\varphi_{\text{in}}(x, 0)S$$

$$\pi_{\text{out}}(x, 0) = S^{-1}\varphi_{\text{out}}(x, 0)S$$

Finally we note that by extending the ideas above one can prove the following abstract result.

Theorem XI.108 Let $\mathscr{H}$ be a separable complex Hilbert space and let $\mathscr{F}_s(\mathscr{H})$ be the boson Fock space over $\mathscr{H}$. For each $f \in \mathscr{H}$, let $a^-(f)$ be the annihilation operator on $\mathscr{F}_s(\mathscr{H})$ defined by (X.62) and set

$$a(f) = a^-(Cf), \qquad a^\dagger(f) = (a^-(f))^*$$

where C is a fixed conjugation on $\mathscr{H}$. Let $\langle B_+, B_- \rangle$ be a pair of bounded linear transformations on $\mathscr{H}$ that satisfy:

$$B_+^* B_+ - B_-^* B_- = I, \qquad B_+^* C B_- = B_-^* C B_+ \tag{298}$$

$$K_+^* K_+ - K_-^* K_- = I, \qquad K_+^* C K_- = K_-^* C K_+ \tag{299}$$

where

$$K_+ = B_+^*, \qquad K_- = -C B_-^* C \tag{300}$$

and set

$$\begin{aligned} a_B(f) &\equiv a^\dagger(CB_- Cf) + a(CB_+ Cf) \\ a_B^\dagger(f) &\equiv a^\dagger(B_+ f) + a(B_- f) \end{aligned} \tag{301}$$

Then there exists a unitary operator W on $\mathscr{F}_s(\mathscr{H})$ so that

$$a_B(f) = W^{-1} a(f) W$$

$$a_B^\dagger(f) = W^{-1} a^\dagger(f) W$$

if and only if B_- is Hilbert–Schmidt. W is uniquely determined up to an overall phase factor.

The mapping $\langle a, a^\dagger \rangle \mapsto \langle a_B, a_B^\dagger \rangle$ given by (301) is called a **Bogoliubov transformation**. The conditions on B_+, B_- are just those needed so that

$$[a_B(f), a_B(g)] = 0 = [a_B^\dagger(f), a_B^\dagger(g)]$$

and

$$[a_B(f), a_B^\dagger(g)] = (Cf, g)_{\mathscr{H}}$$

The K's are the B's for the inverse Bogoliubov transformation and the formulas (299) guarantee invertibility. That is, if (298) and (299) hold, then

$$a^\dagger(f) = a_B^\dagger(K_+ f) + a_B(K_- f)$$

$$a(f) = a_B^\dagger(CK_- Cf) + a_B(CK_+ Cf)$$

XI.16 Quantum field scattering II: The Haag–Ruelle theory

In this section we want to describe scattering ideas in a class of field theories obeying the Wightman axioms of Section IX.8. The free field of Section X.7 will play an important role. In the preceding section we discussed a simple example where the field equation was linear, the interaction was a classical rather than an operator-valued field, and the interaction had compact support in space and time. Even in that case, the construction was nontrivial. How can we hope to construct a scattering theory for a general quantum field theory where none of the above simplifications hold true? The answer is simple. Our construction is axiomatic. We shall assume that the Gårding–Wightman axioms hold; in particular, we assume the existence of a unitary interacting dynamics. It was precisely the construction of such a dynamics that occupied us in the preceding section. Nevertheless, it is striking that the spectrum condition and microcausality conspire in such a way that a scattering theory can be constructed.

The first conceptual problem that must be faced is that there is no natural "free" dynamics for the interacting dynamics to approach as $t \to \pm\infty$. This is of course true in a general axiomatic framework, but it is also true in the types of models introduced in Section X.7 obtained from perturbation of the free field of mass m_0. This is somewhat surprising since one might think that the Hamiltonian H_0 of this free field would play the role of free dynamics. In the first place, the two Hamiltonians act on two different Hilbert spaces for the following reason: When the space cutoff of Section X.7 is removed, one must pass to a new representation of the canonical commutation relations since there is a general result known as Haag's theorem. This theorem asserts that any Wightman field theory in which there are time zero φ's and π's that are unitarily equivalent to those of the free field is the free field theory. Physically significant is the fact that the mass of particles in the interacting theory may not equal m_0; that is, in interacting quantum field theory, unlike classical field theories, the particles can never completely escape their own interaction. These two reasons are connected since, even for the free field, a change in mass means a change in representation of the canonical commutation relations.

In a sense which we shall make precise, the "free dynamics" will be a free field but with the correct physical mass rather than the mass m_0. In this sense there is a similarity to spin-wave scattering in that the comparison dynamics is determined by a piece of the interacting dynamics. The fact that this free field Hamiltonian and the interacting Hamiltonian are naturally given on different Hilbert spaces will be accommodated by the two Hilbert space formalism. However, looking at the Hamiltonians alone is not really satisfactory. For the mass hyperboloid $\{p \mid p \cdot p = m^2\}$ produces absolutely continuous spectrum of infinite multiplicity on $[m, \infty)$. Thus, by looking only at the spectrum of H, one cannot distinguish whether just the hyperboloid is present or whether there are also "multiparticle states." This situation is somewhat improved by looking at the joint energy-momentum spectrum. But the true scattering theory must be connected with the x space behavior of the field $A(x)$ (to avoid confusion, we use Φ for the free field and A for the interacting field).

As a preliminary, let $\Phi_m(x, t)$ be the free field of mass $m > 0$ described in Section X.7. It is clear from (X.84) that for each fixed t, $\Phi_m(\cdot, t)$ and $\dot{\Phi}_m(\cdot, t)$ are operator-valued distributions; the fact that smearing in t is not needed is a special feature of the free field and is not true in general Wightman theories. Let $f(x, t)$ be a regular wave packet for the Klein–Gordon equation $f_{tt} = \Delta f - m^2 f$ of the type defined and discussed in the first appendix to Section 3. Introduce the symbol $\overleftrightarrow{\partial}_0$ to mean

$$\left(g \overleftrightarrow{\partial}_0 k\right)(t) \equiv \int \left[g(x, t) \frac{\partial}{\partial t} k(x, t) - k(x, t) \frac{\partial}{\partial t} g(x, t)\right] d^3x$$

which maps pairs of functions of x and t to a function of t. Then $f \overleftrightarrow{\partial}_0 \Phi_m$ is independent of time since both f and Φ_m obey the Klein–Gordon equation which is second order in time and $f \overleftrightarrow{\partial}_0 \Phi_m$ is essentially a Wronskian. In fact, if the Fourier transform of f in the spatial variables has the form

$$\hat{f}(p, t) = (2\mu(p))^{-1/2} h(p) e^{-i\mu(p)t} \tag{302a}$$

then

$$f \overleftrightarrow{\partial}_0 \Phi_m = i \int h(p) a^\dagger(p)\, d^3p \tag{302b}$$

and if

$$\hat{f}(p, t) = (2\mu(p))^{-1/2} h(p) e^{+i\mu(p)t} \tag{302c}$$

then

$$f \overleftrightarrow{\partial}_0 \Phi_m = -i \int h(-p) a(p)\, d^3p \tag{302d}$$

In particular, (302b) shows that as N runs through 0, 1, …, and f_i runs through all choices obeying (302a), the vectors

$$\left(f_1 \overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\left(f_2 \overset{\leftrightarrow}{\partial}_0 \Phi_m\right) \cdots \left(f_N \overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0$$

run through a total set of $\mathscr{H}_0$, the Hilbert space of the free field.

Suppose that $\langle \mathscr{H}, U, A, D\rangle$ is a Hermitian scalar field obeying the Gårding–Wightman axioms (Properties 1–8 of Section IX.8) and that one has the following two additional properties:

Property 9 (***upper and lower mass gap***) Let P_μ be the generators of the translation subgroup $U(a, I)$ of the Poincaré representation $U(a, \Lambda)$. For some $m > 0$ and some $\varepsilon > 0$, the spectrum of P_μ is contained in

$$\begin{aligned}&\{0\} \cup H_m \cup \bar{V}_{m+\varepsilon,\,+}\\ &\qquad \equiv \{0\} \cup \{p \mid p^2 = m^2;\, p_0 > 0\} \cup \{p \mid p^2 \geq (m+\varepsilon)^2;\, p_0 > 0\}\end{aligned}$$

where $p^2 = p_0^2 - p_1^2 - p_2^2 - p_3^2$. Moreover, the set of vectors $\mathbb{S}$ which are eigenvectors for p^2 with eigenvalue m^2 is nonempty, and there is a cyclic vector for the action of $U(a, I)$ on $\mathbb{S}$.

$\mathbb{S}$ is the family of vectors describing the states of a single spinless particle of mass m. Property 9 ensures that the eigenvalue m^2 is an isolated eigenvalue of P^2.

Property 10 (***coupling of the vacuum to the one particle states***) The spectral weight $d\rho$ for the Källen–Lehmann representation (Theorem IX.34) has the form

$$d\rho(s) = \delta(s - m) + d\tilde{\rho}(s)$$

where $d\tilde{\rho}$ has support in $[m + \varepsilon, \infty)$.

Property 10 essentially says that the vectors $A(f)\psi_0$ where ψ_0 is the vacuum are not all orthogonal to $\mathbb{S}$. For under that condition $d\rho(s) = \alpha\delta(s - m) + d\tilde{\rho}(s)$ with $\alpha \neq 0$. One can then multiply A by a constant so that the new α is 1.

Pick a function h in $C_0^\infty(\mathbb{R})$ so that $h(y)$ is 1 near $y = m^2$ and supp $h \subset (0, m^2 + \varepsilon)$. Define a new operator-valued distribution $B(\mathbf{x}, t)$ by

$$\hat{B}(p) = h(p^2)\hat{A}(p)$$

that is,

$$B(g) = A(Tg) \tag{303}$$

where

$$\widehat{Tg}(p) = h(p^2)\hat{g}(p)$$

Now let $f \in \mathscr{S}(\mathbb{R}^3)$. Then $\hat{f}(\mathbf{p})e^{-ip_0t_0}h(p^2)$ is in $\mathscr{S}(\mathbb{R}^4)$, so we can pick g in (303) to have the form $f(\mathbf{x})\,\delta(t - t_0)$, that is, $B(\mathbf{x}, t)$ is a distribution of $\mathbf{x}$ that is smooth in t, and similarly $\dot{B}(\mathbf{x}, t)$ is a distribution in $\mathbf{x}$. In fact, for $f \in \mathscr{S}(\mathbb{R}^3)$, $B(f, t)$ is C^∞ in t. In particular, for any $f \in C^\infty(\mathbb{R}^4)$ with $f(\cdot, t)$ and $\partial_0 f(\cdot, t)$ in $\mathscr{S}(\mathbb{R}^3)$ for each t, we can form $(f\overset{\leftrightarrow}{\partial}_0 B)(t)$. In general, even if f obeys the Klein–Gordon equation, $(f\overset{\leftrightarrow}{\partial}_0 B)(t)$ is not time independent since B does not obey the Klein–Gordon equation but:

Lemma 1 Let f be a regular wave packet for the mass m Klein–Gordon equation. Then $(f\overset{\leftrightarrow}{\partial}_0 B)(t)\psi_0$ is independent of t where ψ_0 is the vacuum for the theory.

Proof In general, $B(x)$ does not obey the Klein–Gordon equation, but $B(x)\psi_0$ does. ▌

By Property 10,

$$\left(\left(f\overset{\leftrightarrow}{\partial}_0 B\right)\psi_0, \left(g\overset{\leftrightarrow}{\partial}_0 B\right)\psi_0\right) = \left(\left(f\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0, \left(g\overset{\leftrightarrow}{\partial}_0 \Phi_m\right)\Omega_0\right) \tag{304}$$

For the left-hand side of (304) can be written in terms of the two point function for A. Since B has built into it a factor of $h(p^2)$, Property 10 says that only the $\delta(s - m)$ term from the spectral weight survives. What is left is then the same thing that would occur if A were equal to Φ_m. Since $\hat{\Phi}_m(p) = h(p^2)\hat{\Phi}_m(p)$, (304) holds.

The main theorem of the Haag–Ruelle theory is the following:

Theorem XI.109 Let A be a Hermitian scalar field theory obeying the Gårding–Wightman axioms (Properties 1–8) and also Properties 9 and 10. Define B as above. Then:

(a) For any regular wave packets $f^{(1)}, \ldots, f^{(n)}$, the limits

$$\lim_{t \to \mp\infty} \left(f^{(1)}\overset{\leftrightarrow}{\partial}_0 B\right)(t) \cdots \left(f^{(n)}\overset{\leftrightarrow}{\partial}_0 B\right)(t)\psi_0 \equiv \eta_{\substack{\text{in}\\\text{out}}}(f^{(1)}, \ldots, f^{(n)})$$

exist in the norm topology on $\mathscr{H}$ and are independent of the choice of h. Let $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ denote the closed span of the η_{in} and the η_{out}.

(b) $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ are left invariant by the representation U of the Poincaré group.

(c) There are operator-valued distributions φ_{in} on $\mathscr{H}_{\text{in}}$ and φ_{out} on $\mathscr{H}_{\text{out}}$ so that $\langle \mathscr{H}_{\text{in}}, U, \varphi_{\text{in}} \rangle$ and $\langle \mathscr{H}_{\text{out}}, U, \varphi_{\text{out}} \rangle$ are unitarily equivalent to the free field of mass m and so that

$$\eta_{\substack{\text{in}\\ \text{out}}}(f^{(1)}, \ldots, f^{(n)}) = \left(f^{(1)} \overleftrightarrow{\partial}_0 \varphi_{\substack{\text{in}\\ \text{out}}}\right) \cdots \left(f^{(n)} \overleftrightarrow{\partial}_0 \varphi_{\substack{\text{in}\\ \text{out}}}\right) \psi_0$$

Before discussing the physical interpretation of this theorem and its proof, we note a mathematical consequence analogous to the spectral implications of the existence of wave operators in ordinary quantum mechanics. Since U restricted to $\mathscr{H}_{\text{in}}$ is unitarily equivalent to the U of the free field, we have:

Corollary 1 In a field theory obeying Properties 1–10, the energy momentum spectrum contains $\{p \mid p^2 \geq (2m)^2;\ p_0 > 0\}$.

In particular, one has the striking fact that one cannot construct a Wightman field theory with $\sigma(P) = \{p \mid p^2 = m^2,\ p_0 > 0\} \cup \{0\}$!

To help illustrate the scattering theoretic content of Theorem XI.109, one can either attempt to rewrite it in terms of some kind of wave operator or one can attempt to rephrase the usual nonrelativistic framework into a form similar to Theorem XI.109. We follow the former course here and leave the latter to the references in the Notes and problems (Problem 142). Let $f^{(1)}, \ldots, f^{(n)}$ obey (302a). Define a map J from a dense subset of $\mathscr{H}_0$, the Hilbert space for the free field of mass m, to $\mathscr{H}$ by

$$J\left[\prod_{i=1}^{n} \left(f^{(i)} \overleftrightarrow{\partial}_0 \Phi_m\right) \Omega_0\right] = \prod_{i=1}^{n} \left(f^{(i)} \overleftrightarrow{\partial}_0 B\right)(t = 0) \psi_0$$

J is well defined because a given vector $\psi \in \mathscr{H}_0$ can be written in at most one way as

$$\psi = \prod_{i=1}^{n} \left(f^{(i)} \overleftrightarrow{\partial}_0 \Phi_m\right) \Omega_0$$

if the $f^{(i)}$ are required to satisfy (302a). It is because of the requirement that J be well defined that we cannot use the more natural formula

$$J\left[\prod_{i=1}^{n} (\Phi_m(g^{(i)}))\, \Omega_0\right] = \left[\prod_{i=1}^{n} A(g^{(i)})\right] \psi_0$$

Let $\mathscr{D}_0$ be the set of vectors of the form $\prod_{i=1}^n (f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m)\Omega_0$ which is total in $\mathscr{H}_0$ by (302b). Then:

Corollary 2 $\Omega^\pm = \text{s-lim}_{t\to\mp\infty} e^{itH}Je^{-itH_0}$ exist and define partial isometries $\mathscr{H}_0 \xrightarrow{\Omega^+} \mathscr{H}_{\text{in}}$ and $\mathscr{H}_0 \xrightarrow{\Omega^-} \mathscr{H}_{\text{out}}$.

Proof Let $e^{-ith_0}f$ be defined by

$$(e^{-ith_0}f)(x, s) = f(x, t+s)$$

Then

$$e^{-itH_0}\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 = \prod_{i=1}^n \left[e^{-ith_0}f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0$$

so

$$\begin{aligned} e^{itH}Je^{-itH_0}\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 &= \prod_{i=1}^n e^{itH}\left(f^{(i)}(\cdot, t)\overleftrightarrow{\partial}_0 B(\cdot, 0)\right)e^{-itH}\psi_0 \\ &= \prod_{i=1}^n \left(f^{(i)}\overleftrightarrow{\partial}_0 B\right)(t)\psi_0 \end{aligned}$$

so by Theorem XI.109, the limits defining $\Omega^\pm$ exist and

$$\Omega^\pm\left[\prod_{i=1}^n f^{(i)}\overleftrightarrow{\partial}_0 \Phi_m\right]\Omega_0 = \prod_{i=1}^n (f^{(i)}\overleftrightarrow{\partial}_0 \varphi_{\substack{\text{in}\\\text{out}}})\psi_0 \tag{305}$$

By (c) of the theorem, $\Omega^\pm$ are isometries. ▌

(305) says that

$$\Omega^\pm\Phi_m = \varphi_{\substack{\text{in}\\\text{out}}}\Omega^\pm$$

In particular, the Jauch S-matrix $S = \Omega^+(\Omega^-)^*$ obeys

$$\varphi_{\text{out}} = S^{-1}\varphi_{\text{in}}S$$

if we have the condition of *asymptotic completeness*

$$\mathscr{H}_{\text{in}} = \mathscr{H}_{\text{out}} = \mathscr{H} \tag{306}$$

It certainly happens that (306) fails in some models, for example, in many generalized free fields (see the Notes to Section IX.8). One hopes that this is due to the artificiality of the models and that real models will obey asymptotic completeness, at least if one can construct asymptotic fields for each discrete mass hyperboloid and build the corresponding states with all possible asymptotic particles. For this reason, in further developments, (306) is often taken as an axiom.

We now turn to the proof of Theorem XI.109. It depends on four facts. The first is Lemma 1; the second is the falloff of regular wave packets for the Klein–Gordon equation as summarized in Theorem XI.17 and its corollary. To describe the third we need to introduce the notion of truncated vacuum expectation value (TVEV).

Definition A **partition** of the ordered set $\langle 1, \ldots, n\rangle$ is a family P of ordered subsets $S_1 = \langle i_1, \ldots, i_{k(1)}\rangle, \ldots, S_\ell = \langle i'_1, \ldots, i'_{k(\ell)}\rangle$ so that $i_1 < \cdots < i_{k(1)}, \ldots, i'_1 < \cdots < i'_{k(\ell)}$ and so that $\bigcup S_j = \langle 1, \ldots, n\rangle$ and $S_j \cap S_q = \emptyset$. $\mathscr{P}_n$ will denote the set of all partitions of $\langle 1, \ldots, n\rangle$.

Definition The **truncated vacuum expectation values** of a Wightman theory are the distributions $\mathscr{W}_{n,\mathrm{T}}$ defined in terms of the Wightman distributions $\mathscr{W}_n$ by the relation

$$\mathscr{W}_n(x_1, \ldots, x_n) = \sum_{P \in \mathscr{P}_n} \mathscr{W}_{k(1),\mathrm{T}}(x_{i_1}, \ldots, x_{i_{k(1)}}) \cdots \mathscr{W}_{k(\ell),\mathrm{T}}(x_{i_{\ell'}}, \ldots, x_{i_{k(\ell)'}}) \tag{307}$$

Clearly, the $\mathscr{W}_{n,\mathrm{T}}$ are defined inductively from (307) since if $\mathscr{W}_{1,\mathrm{T}}, \ldots, \mathscr{W}_{n-1,\mathrm{T}}$ are defined, then exactly one term on the right of (307), namely the one with $P = \{\langle 1, \ldots, n\rangle\}$ is not previously defined and so is defined by (307). The first few $\mathscr{W}_{n,\mathrm{T}}$ are given by

$$\begin{aligned}
\mathscr{W}_{1,\mathrm{T}}(x_1) &= (\psi_0, \varphi(x_1)\psi_0)\\
\mathscr{W}_{2,\mathrm{T}}(x_1, x_2) &= (\psi_0, \varphi(x_1)\varphi(x_2)\psi_0)\\
&\quad - (\psi_0, \varphi(x_1)\psi_0)(\psi_0, \varphi(x_2)\psi_0)\\
\mathscr{W}_{3,\mathrm{T}}(x_1, x_2, x_3) &= \mathscr{W}_3(x_1, x_2, x_3) - \mathscr{W}_1(x_1)\mathscr{W}_2(x_2, x_3)\\
&\quad - \mathscr{W}_1(x_2)\mathscr{W}_2(x_1, x_3)\\
&\quad - \mathscr{W}_1(x_3)\mathscr{W}_2(x_1, x_2) + 2\mathscr{W}_1(x_1)\mathscr{W}_1(x_2)\mathscr{W}_1(x_3)
\end{aligned}$$

There are a variety of explicit formulas for $\mathscr{W}_{n,\mathrm{T}}$ (see the Notes and Problem 143) but the implicit formulas (307) are all that we shall need. The reason that the $\mathscr{W}_{n,\mathrm{T}}$ are natural is the following fact which we will eventually prove: Since $\mathscr{W}_{n,\mathrm{T}}$ is translation invariant, we can form $W_{n,\mathrm{T}}(\zeta_1, \ldots, \zeta_{n-1})$ as in Section IX.8. Under the spectral hypothesis, Property 9, $\hat{W}_n$

has support in $\times_{j=1}^{n-1} (-\bar{V}_{m,+} \cup \{0\})$; $\hat{W}_{n,\mathrm{T}}$ has support only in $\times_{j=1}^{n-1} (-\bar{V}_{m,+})$. In particular, the supports of the Fourier transform of $W_{n,\mathrm{T}}(\zeta_1, \ldots, \zeta_{n-1})$ and $W_{n,\mathrm{T}}(-\zeta_{n-1}, \ldots, -\zeta_1)$ will be disjoint, which will be important.

The third basic fact needed in the proof of Theorem XI.109 is the following:

Theorem XI.110 (cluster property of TVEV) Fix $f \in \mathscr{S}(\mathbb{R}^{4n})$. For $a_1, \ldots, a_n \in \mathbb{R}^3$, let

$$F(a_1, \ldots, a_n) = \int_{\mathbb{R}^{4n}} \mathscr{W}_{n,\mathrm{T}}(x_1, \ldots, x_n) f(x_1 - a_1, \ldots, x_n - a_n)\, dx_1 \cdots dx_n \tag{308}$$

(where a_i is used for $\langle a_i, 0 \rangle \in \mathbb{R}^4$). Define G by

$$G(\alpha_1, \ldots, \alpha_{n-1}) = F(a_1, \ldots, a_n); \qquad \alpha_i = a_{i+1} - a_i$$

Then $G \in \mathscr{S}(\mathbb{R}^{3n-3})$.

The last result required for the proof of Theorem XI.109 is:

Theorem XI.111 Let K be a distribution in $\mathscr{S}'(\mathbb{R}^\nu)$ so that $K * f \in \mathscr{S}(\mathbb{R}^\nu)$ for every $f \in \mathscr{S}(\mathbb{R}^\nu)$. Then, for any N, there is a constant coefficient differential operator $P(D)$, and a continuous function F on $\mathbb{R}$ so that

$$K = P(D)F$$

$$|F(x)| \leq C(1 + x^2)^{-N}$$

We turn now to the proof of Theorem XI.109. Theorems XI.110 and XI.111 are proven later in the section.

Proof of Theorem XI.109 Introduce the symbol $B_f(t)$ for $f(\cdot, t)\overleftrightarrow{\partial_0} B(\cdot, t)$. Let $C_1(t), \ldots, C_n(t)$ be n operators each of which is either a $B_f(t)$ or a time derivative of a $B_f(t)$. Let $(\psi_0, C_1(t) \cdots C_n(t)\psi_0)_T$ denote a truncated expectation as defined above. We first claim that

$$|(\psi_0, C_1(t) \cdots C_n(t)\psi_0)_T| \leq c(1 + |t|)^{-\frac{3}{2}(n-2)} \tag{309}$$

To prove (309), we first expand the C's as sums of $B(x, t)$'s smeared with f's. The new f's are all regular wave packets for the Klein–Gordon equation since they are the original f's or their time derivatives. Thus the left-hand side of (309) is bounded by a sum of terms of the form

$$\left| \int f^{(1)}(x_1, t) \cdots f^{(n)}(x_n, t)(\psi_0, Q_1(x_1, t) \cdots Q_n(x_n, t)\psi_0)_T \, d^{3n}x \right| \tag{310}$$

where each Q is B, $\partial_0 B$ or $\partial_0^2 B$. Define $K(\zeta_1, \ldots, \zeta_{n-1})$ by

$$K(\zeta_1, \ldots, \zeta_{n-1}) = (\psi_0, Q_1(x_1, t) \cdots Q_n(x_n, t)\psi_0)_T; \qquad \zeta_i = x_{i+1} - x_i$$

$K \in \mathscr{S}'(\mathbb{R}^{3n-3})$ and is independent of t by the time translation covariance of the theory. By (303), K smeared with a g in $\mathscr{S}(\mathbb{R}^{3n-3})$ can be rewritten as $W_{n,\mathrm{T}}$ smeared with a $\tilde{g}$ in $\mathscr{S}(\mathbb{R}^{4n-4})$; so by Theorem XI.110, $K * g \in \mathscr{S}(\mathbb{R}^{3n-3})$ for each g in $\mathscr{S}(\mathbb{R}^{3n-3})$. Thus, by Theorem XI.111, we can find a differential operator $P(D)$ and continuous function F so that $K = P(D)F$ and

$$|F(\zeta_1, \ldots, \zeta_{n-1})| \le C(1 + |\zeta|^2)^{-3n}$$

Therefore, (310) can be dominated by a sum of terms of the form

$$C \left| \int g_1(x_1, t) \cdots g_n(x_n, t)(1 + |\zeta|^2)^{-3n} \, d^{3n}x \right| \tag{311}$$

where each g_i is a derivative of an $f^{(i)}$ and thus a regular wave packet for the Klein–Gordon equation. As a result, by the corollary to Theorem XI.17,

$$|g_2(x_2, t)| \le c_2(1 + |t|)^{-\frac{3}{2}}, \ldots, |g_n(x_n, t)| \le c_n(1 + |t|)^{-\frac{3}{2}}$$

$$\int |g_1(x_1, t)| \, d^3x_1 \le c_1(1 + |t|)^{\frac{3}{2}}$$

so that (311) is dominated by

$$c(1 + |t|)^{-\frac{3}{2}(n-1)} \int |g_1(x, t)| (1 + |\zeta|^2)^{-3n} \, d^{3n}x \le d(1 + |t|)^{-\frac{3}{2}(n-2)}$$

This proves (309).

Using (309), we can prove that the limit in Theorem XI.109 (a) exists by a modified Cook argument. Let

$$\eta(t) = B_{f^{(1)}}(t) \cdots B_{f^{(n)}}(t)\psi_0$$

We shall prove that

$$\left\| \frac{d\eta}{dt} \right\| \le c(1 + |t|)^{-\frac{3}{2}} \tag{312}$$

so that $\lim_{t \to \mp\infty} \eta(t)$ exists. Clearly $\|d\eta/dt\|^2$ is a sum of $(\psi_0, C_1(t) \cdots C_{2n}(t)\psi_0)$ terms and thus a sum of products of $(\psi_0, C_{i_1}(t) \cdots C_{i_k}(t)\psi_0)_T$. Since $(\psi_0, B(x, t)\psi_0) = 0$, none of the products has one-point TVEV's. Each product is one of the following types:

(1) One of the factors is an m-point TVEV with $m \geq 4$. By (309), this factor is bounded by $(1 + |t|)^{-3}$.
(2) No factor is an m-point TVEV with $m \geq 4$, but at least one three-point TVEV occurs. In this case, since $2n$ is even, at least two such factors must occur, each with $(1 + |t|)^{-3/2}$ falloff, so again the overall falloff is at least $(1 + |t|)^{-3}$.
(3) All the factors are two-point functions. In this case one of the factors must be of the form

$$\left(\psi_0, B_{f^{(1)}}(t)\frac{dB_{f^{(2)}}}{dt}(t)\psi_0\right) \qquad \text{or} \qquad \left(\psi_0, \frac{dB_{f^{(1)}}(t)}{dt}\,\frac{dB_{f^{(2)}}(t)}{dt}\psi_0\right)$$

or

$$\left(\psi_0, \frac{dB_{f^{(1)}}}{dt}(t)B_{f^{(2)}}(t)\psi_0\right) = \left(\frac{dB_{\overline{f^{(1)}}}}{dt}(t)\psi_0, B_{f^{(2)}}(t)\psi_0\right)$$

which all vanish, by Lemma 1. Thus such products vanish.

We therefore see that $\|d\eta/dt\|^2 \leq C(1 + |t|)^{-3}$ proving (312) and so part (a) of the theorem.

The invariance of $\mathscr{H}_{\text{in}}$ and $\mathscr{H}_{\text{out}}$ under space–time translations is obvious. The invariance under Lorentz transformations and the independence of the limits of the choice of h are discussed in the references in the Notes.

Motivated by (302), we define $a_{\text{in}}(p)$ and $a_{\text{in}}^\dagger(p)$ by

$$\left(i \int h(p)a_{\text{in}}^\dagger(p)\, d^3p\right)(\eta_{\text{in}}(f^{(2)}, \ldots, f^{(n)})) = \eta_{\text{in}}(f^{(1)}, \ldots, f^{(n)})$$

where h and $f^{(1)}$ are related by (302a) and similarly for $a_{\text{in}}(p)$ using (302c). φ_{in} is then defined using (X.85). The covariance of φ_{in} and φ_{out} under space–time translations is immediate; and, again, the Lorentz covariance can be found in the references. The unitary equivalence of φ_{in} to the free field Φ_m is given by

$$V(\eta_{\text{in}}(f^{(1)}, \ldots, f^{(n)})) = \left[\prod_{i=1}^{n}\left(f^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\right]\Omega_0$$

To check that V is well defined and unitary we need only prove that

$$\begin{aligned}(\eta_{\text{in}}(f^{(1)}, \ldots, f^{(m)}), \eta_{\text{in}}(g^{(1)}, \ldots, g^{(n)}))\\ = \left(\left(\prod_{i=1}^{m} f^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\Omega_0, \left(\prod_{i=1}^{n} g^{(i)}\overleftrightarrow{\partial}_0\Phi_m\right)\Omega_0\right)\end{aligned} \tag{313}$$

It is then easy to check that

$$V\varphi_{\text{in}}V^{-1} = \Phi_m$$

The left-hand side of (313) is the limit of $(\prod B_{f^{(i)}}\psi_0, \prod B_{g^{(i)}}(t)\psi_0)$ as $t \to -\infty$. Expanding this product as a sum of TVEV's, those terms with some m-point TVEV with $m \ge 3$ vanish by (309). The only terms remaining as $t \to -\infty$ are products of two-point functions which, by Lemma 1, are time independent as we have explained. And, by Property 10, these are identical to the two point function for Φ_m; See (304). Since the n-point function of the free field is a sum of products of two-point functions (see (X.162)), (313) holds. ▮

Proof of Theorem XI.111 By the closed graph theorem $f \mapsto K * f$ is continuous. Let $T = \hat{K}$. Then, by hypothesis and $\widehat{K * f} = (2\pi)^{\nu/2}\hat{K}\hat{f}$ (Theorem IX.4), gT is in $\mathscr{S}(\mathbb{R}^\nu)$ for any $g \in \mathscr{S}(\mathbb{R}^\nu)$. It follows that T is a C^∞ function each of whose derivatives is of polynomial growth, that is, $T \in \mathcal{O}_M$ (see Problem 23 of Chapter V). Given N, pick k so that for all α with $|\alpha| \le 2N$,

$$|(D^\alpha T)(x)| \le c(1 + x^2)^k$$

Now let $G(x) = (1 + x^2)^{-k-\nu}T(x)$. Then for $|\alpha| \le 2N$,

$$|(D^\alpha G)(x)| \le c(1 + x^2)^{-\nu}$$

Thus since each $D^\alpha G$ is in L^1, $F = \check{G}$ is a distribution which is a bounded continuous function with $x^\alpha F(x)$ bounded for each $|\alpha| \le 2N$. Therefore

$$|F(x)| \le c(1 + x^2)^{-N}$$

and $K = (1 - \Delta)^{k+\nu}F$. ▮

We now begin the proof of Theorem XI.110. We first need to establish that $\hat{W}_{n,T}$ has support in $(-\bar{V}_{m,+})^{(n-1)}$.

Lemma 2 Let a be a spacelike vector in $\mathbb{R}^4$. Then

$$\lim_{\lambda\to\infty} \mathscr{W}_n(x_1, \ldots, x_i, x_{i+1} + \lambda a, \ldots, x_n + \lambda a)$$
$$= \mathscr{W}_i(x_1, \ldots, x_i)\mathscr{W}_{n-i}(x_{i+1}, \ldots, x_n)$$

in the sense that for any $f \in \mathscr{S}(\mathbb{R}^{4i})$, $g \in \mathscr{S}(\mathbb{R}^{4(n-i)})$,

$$\mathscr{W}_n(f \otimes g_\lambda) \to \mathscr{W}_i(f)\mathscr{W}_{n-i}(g) \tag{314}$$

as $\lambda \to \infty$ where

$$(f \otimes g_{\lambda a})(x_1, \ldots, x_n) = f(x_1, \ldots, x_i)g(x_{i+1} - \lambda a, \ldots, x_n - \lambda a)$$

Moreover, the Fourier transform of $W_n(\zeta_1, \ldots, \zeta_{n-1})$ is a (signed) measure in the p_i variable (when smeared in the other variables) and

$$\hat{W}_n(p_1, \ldots, p_{n-1}) = (2\pi)^2 \hat{W}_i(p_1, \ldots, p_{i-1})\hat{W}_{n-i}(p_{i+1}, \ldots, p_{n-1})\delta(p_i) + R(p) \tag{315}$$

where, after smearing in the other variables, R is a measure in p_i assigning zero weight to $p_i = 0$.

Proof Fix $f \in \mathscr{S}(\mathbb{R}^{4i})$, $g \in \mathscr{S}(\mathbb{R}^{4(n-i)})$. Let

$$\psi_1 = \int \overline{f(x_1, \ldots, x_i)}\varphi(x_i) \cdots \varphi(x_1)\psi_0 \, dx_1 \cdots dx_i$$

and

$$\psi_2 = \int g(x_1, \ldots, x_{n-i})\varphi(x_1) \cdots \varphi(x_{n-i})\psi_0 \, dx_1 \cdots dx_{n-i}$$

Then, as in the proof of Theorem IX.32, if $g_a(x) = g(x_1 - a, \ldots, x_{n-i} - a)$,

$$\mathscr{W}_n(f \otimes g_a) = \int_{\mathbb{R}^4} e^{ik \cdot a} \, d(\psi_1, E_{\tilde{k}}\psi_2)$$

where E_Ω is the spectral measure for the energy–momentum and $\tilde{k} = \langle k_0, -\mathbf{k} \rangle$. By uniqueness of the vacuum

$$d(\psi_1, E_{\tilde{k}}\psi_2) = (\psi_1, \psi_0)(\psi_0, \psi_2)\delta(\tilde{k}) + R(\tilde{k})$$

From this, (315) follows immediately. (314), which is not used below, is left to the problems (Problem 145). ▮

Lemma 3 For fields obeying Property 9, $\hat{W}_{n, T}$ has support in $(-\bar{V}_{m,+})^{(n-1)}$, $n \geq 2$.

Proof As in the proof of Theorem IX.32, by Property 9, $\hat{W}_n$ has support in $(\{0\} \cup (-\bar{V}_{m,+}))^{n-1}$. $\hat{W}_{n,T}$ clearly has the same property. Moreover, $\hat{W}_{n,T}$ is a measure in each variable as in Lemma 2. Thus, we need only prove that when smeared in all variables except p_i, $\hat{W}_{n,T}$ has no $\delta(p_i)$ contribution. The proof is by induction on n. For $n = 2$, $W_{2,T}(x) = W_2(x) - W_1^2$ so

$$\hat{W}_{2,T}(p) = \hat{W}_2(p) - (2\pi)^2\delta(p)W_1^2$$

so, by (315), the $\delta(p)$ contribution to $\hat{W}_{2,\mathrm{T}}$ is zero. Now suppose by induction that $\hat{W}_{j,\mathrm{T}}$ has support in $(-\bar{V}_{m,+})^{(j-1)}$ for $j = 2, \ldots, n-1$. Fix i and consider

$$\hat{\mathscr{W}}_{n,\mathrm{T}} = \hat{\mathscr{W}}_n - \sum_{\substack{P\in\mathscr{P}_n\\ P\neq\{1,\ldots,n\}}} \Bigl(\prod_{S_j\in P} \mathscr{W}_{S_j,\mathrm{T}}\Bigr)^{\wedge}$$

Break the sum over $\mathscr{P}_n$ into two pieces. The first is those P's where it never happens that some $k_1 \le i$ and $k_2 \ge i+1$ are in the same subset $S_j \in P$. Clearly the sum over such P's yields the Fourier transform of $\mathscr{W}_i(x_1, \ldots, x_i)\mathscr{W}_{n-i}(x_{i+1}, \ldots, x_n)$ so the contribution of this sum to $\hat{W}_{n,\mathrm{T}}(p)$ precisely cancels the $\delta(p_i)$ part of $\hat{W}_n$. In the second piece of the sum, p_i is a sum of momenta in the $\hat{W}_{S_j,\mathrm{T}}$ and thus, by the induction hypothesis, this sum has p_i support in $(-\bar{V}_{m,+})$ (see Problem 146). It follows that $\hat{W}_{n,\mathrm{T}}(p)$ has no $\delta(p_i)$ contribution, so its support is in $(-\bar{V}_{m,+})^{(n-1)}$. ∎

Proof of Theorem XI.110 Since the function F of (308) has the property that derivatives of F are again of the same form, we need only show that for any N,

$$\sup_{\alpha} d(\alpha)^N F(a_1, \ldots, a_n) < \infty \tag{316}$$

where $d(\alpha) = (\sum_{i=1}^{n-1} (a_{i+1} - a_i)^2)^{1/2}$. Clearly, it suffices to show that for any unit vector $\hat{\alpha}$ in $\mathbb{R}^{3n-3}$, (316) holds uniformly for $\alpha/\|\alpha\|$ in some fixed neighborhood of $\hat{\alpha}$. Given $\hat{\alpha}$, we first claim that we can find a partition of $\langle 1, \ldots, n\rangle$ into two sets $I = \{i_1, \ldots, i_k\}$ and $I' = \{i'_1, \ldots, i'_{n-k}\}$ so that if $a_{i+1} - a_i = \hat{\alpha}_i$, then $\|a_j - a_{i'}\| \ge n^{-3/2}$ for all $j \in I$ and i' in I'. This follows from the following argument: Some component of $\hat{\alpha}$, say $\hat{\alpha}_j$, must have length at least $n^{-1/2}$. Consider the n planes in $\mathbb{R}^3$ perpendicular to $a_{j+1} - a_j$ through the a_i. Clearly some pair of adjacent planes must be a distance apart at least $n^{-1}\|a_{j+1} - a_j\| \ge n^{-3/2}$. Take I to be those points on one side of the pair of planes and I' on the other. Pick a neighborhood M about $\hat{\alpha}$ so that if $\alpha/\|\alpha\| \in M$, then for all $j \in I$ and $i' \in I'$,

$$\|a_j - a_{i'}\| \ge \frac{1}{2n^{3/2}} \|\alpha\|$$

Let $\tilde{M} = \{\alpha \neq 0 \mid \alpha/\|\alpha\| \in M\}$. We shall prove that (316) holds for $\alpha \in \tilde{M}$. Since the unit sphere can be covered by finitely many M's, (316) will then follow. Define

$$\mathscr{W}'_{n,\mathrm{T}}(x_1, \ldots, x_n) = \mathscr{W}_{n,\mathrm{T}}(x_{i_1}, \ldots, x_{i_k}, x_{i'_1}, \ldots, x_{i'_{n-k}})$$

$$\mathscr{W}''_{n,\mathrm{T}}(x_1, \ldots, x_n) = \mathscr{W}_{n,\mathrm{T}}(x_{i'_1}, \ldots, x_{i'_{n-k}}, x_{i_1}, \ldots, x_{i_k})$$

where we order I and I' so that $i_1 < \cdots i_k$; $i'_1 < \cdots < i'_{n-k}$. We claim that, for any N, and any $g \in \mathscr{S}(\mathbb{R}^{4n})$,

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)(\mathscr{W}'_{n,\mathrm{T}}(g_a) - \mathscr{W}_{n,\mathrm{T}}(g_a))| < \infty \tag{317a}$$

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)(\mathscr{W}''_{n,\mathrm{T}}(g_a) - \mathscr{W}_{n,\mathrm{T}}(g_a))| < \infty \tag{317b}$$

Accepting (317) for the time being, let us prove (316) for $\alpha \in \tilde{M}$. Let S' (respectively, S'') be the support of $\mathscr{W}'$ (respectively, supp $\mathscr{W}''$). If $\langle p_1, \ldots, p_n \rangle \in S'$ (respectively, S''), then by Lemma 3 and Problem 146, $P = \sum_{i \in \alpha} p_i$ lies in $-\bar{V}_{m,+}$ (respectively, $\bar{V}_{m,+}$). Let h be a bounded C^∞ function with bounded derivatives so that $h = 1$ on $-\bar{V}_{m,+}$ and $h = 0$ on $\bar{V}_{m,+}$. Let $g = (h\hat{f})^\vee$. Then $\mathscr{W}''_{n,\mathrm{T}}(g_a) = 0$ and $\mathscr{W}'_{n,\mathrm{T}}(g_a) = \mathscr{W}'_{n,\mathrm{T}}(f_a)$. Thus, by (317), $\sup_{\alpha \in \tilde{M}} |d^N(\alpha)\mathscr{W}'_{n,\mathrm{T}}(f_a)| < \infty$. Using (317a) again

$$\sup_{\alpha \in \tilde{M}} |d^N(\alpha)\mathscr{W}_{n,\mathrm{T}}(f_a)| < \infty.$$

This proves (316).

Thus, we need only prove (317) to complete the proof. Let $\alpha \in M$ be fixed and let $x \in \mathbb{R}^{4n}$ be such that $\|x\| < d(\alpha)/4n^{3/2}$. Then for any $j \in I$, $i' \in I'$,

$$\begin{aligned} \|x_j - x_{i'}\|^2 &\le 2(\|x_{i'}\|^2 + \|x_j\|^2) \\ &\le 2\|x\|^2 < \tfrac{1}{2}(d(\alpha)/2n^{3/2})^2 \\ &\le \tfrac{1}{2}\|a_j - a_{i'}\|^2 \end{aligned}$$

Letting $\zeta = x_{i'} - x_j \in \mathbb{R}^4$ and $\alpha = a_{i'} - a_j \in \mathbb{R}^3$, we have

$$\zeta_0^2 + \zeta^2 < \tfrac{1}{2}\|\alpha\|^2$$

so

$$(|\zeta_0| + |\zeta|)^2 \le 2\zeta_0^2 + 2|\zeta|^2 < \|\alpha\|^2$$

or

$$|\zeta_0| < \|\alpha\| - \|\zeta\| \le \|\alpha + \zeta\|$$

Thus $\zeta + \alpha$ is spacelike, that is, if $\|x\| < d(\alpha)/4n^{3/2}$, $\alpha \in \tilde{M}$ and $j \in I$, $i' \in I'$, then the $(x + a)_{i'}$ and $(x + a)_j$ are spacelike separated. It follows by local commutativity that for such x,

$$\mathscr{W}'_{n,\mathrm{T}}(x + a) = \mathscr{W}_{n,\mathrm{T}}(x + a)$$

Thus for any $h_{(a)}$ in C^∞ which is 1 for $\|x\| \ge d(\alpha)/4n^{3/2}$,

$$|\mathscr{W}_{n,\mathrm{T}}(g_a) - \mathscr{W}'_{n,\mathrm{T}}(g_a)| \le |\mathscr{W}^{(a)}_{n,\mathrm{T}}(gh_{(a)})| + |\mathscr{W}^{(a)}_{n,\mathrm{T}}(gh_{(a)})| \tag{318}$$

where $\mathscr{W}^{(a)}(x) = \mathscr{W}(x + a)$. We can pick $h_{(a)}$ vanishing on the set of those x with $\|x\| \le d(\alpha)/8n^{3/2}$ and so that for $d(\alpha) \ge 1$, the norms $\|D^\beta h_{(a)}\|$ are uniformly bounded in a. By the regularity theorem for tempered distributions, there is some differential operator $P(D)$ and some continuous function F obeying

$$|F(x)| \le c(1 + x^2)^N$$

so that $\mathscr{W}_{n,\mathrm{T}} = P(D)F$. Thus

$$\begin{aligned} |\mathscr{W}^{(a)}_{n,\mathrm{T}}(gh_{(a)})| &\le c_0 \int (1 + (x + a)^2)^N |P(D)(gh_{(a)})| \, dx \\ &\le c(1 + a^2)^N \int (1 + x^2)^N |P(D)(gh_{(a)})(x)| \, dx \end{aligned}$$

Because of the falloff of g and the support properties of $h_{(a)}$, the integral above goes to zero faster than any power of $d(\alpha)$. Thus (317a) follows from (318) if we note that, for any α, we can choose a corresponding a satisfying $a^2 \le C\, d(\alpha)^2$, say, by taking $a_1 = 0$. The proof of (317b) is similar. ▌

XI.17 Phase space analysis of scattering and spectral theory

> *The first step of the proof is to wait. It may take a long time for the particle to move far from the scatterer. We need patience. After all, think how long we had to wait for a proof of asymptotic completeness.*
>
> *V. Enss*

In this section we describe a remarkable approach to studying the basic completeness and spectral problems for Schrödinger operators. The method has potentialities for multiparticle systems. We present the two-body problem where, modulo some logarythmic differences in hypotheses, the results for local potentials are very similar to the Agmon–Kato–Kuroda theorem (Theorem XIII.33) proven in Section XIII.8. The methods, however, are strikingly different: the latter theory depends on considerable, albeit elegant, machinery, including restricting Fourier transforms to spheres (Section IX.9), the theory of locally smooth perturbations (Section XIII.7), and the analytic Fredholm theory (Section VI.5). In comparison, this section will use little more than Cook's method, integration by parts (in the context of Theorem XI.14), and one critical piece of physical insight: any state that is not bound will have to spend long times away from the scatterer (this is made precise by the RAGE theorem which we prove in an appendix to this section) and at those times the potential should be negligible. If we decompose the state at that time into two pieces, one with velocities pointing away from the scattering center and one pointing toward the scattering center, then one piece should not interact appreciably in the future, and the other should not interact appreciably in the past.

Throughout our discussion of the two-body problem we let $H_0 = -\frac{1}{2}\Delta$. This choice of $m = 1$ is convenient since velocities are then identical to momenta. We let $F(S)$ denote the operator that is multiplication by the characteristic function of S.

Definition A symmetric operator V on $L^2(\mathbb{R}^\nu)$ is said to be an **Enss potential** if and only if

(a) V is a relatively bounded perturbation of H_0 with relative bound $a < 1$.
(b) The function h on $[0, \infty)$ given by

$$h(R) = \|V(H_0 + i)^{-1}F(|x| \geq R)\|$$

is in $L^1(0, \infty; dR)$. $h(R)$ is automatically monotone decreasing so

$$\lim_{R \to \infty} h(R) = 0$$

Notice that we do not require V to be a multiplication operator; but if V is such an operator, one can show (Problem 151d) that $h(R)$ is in L^1 if and only if

$$h(R) = \|F(|x| \geq R)V(H_0 + i)^{-1}\|$$

is in L^1. In particular, if V is a multiplication operator with $(1 + |x|)^{1+\varepsilon}V(H_0 + i)^{-1}$ bounded and if V has H_0-relative bound smaller than 1, then V is an Enss potential.

To show how natural the Enss condition is let us begin by showing that if V is an Enss potential, then the wave operators exist. Let f be a function in $\mathcal{S}(\mathbb{R}^\nu)$ such that $\hat{f}$ has compact support in $\{k \mid |k| > a\}$. By the corollary to Theorem XI.14

$$|(e^{-itH_0}(H_0 + i)f)(x)| \leq C(1 + |x| + |t|)^{-\nu-1}, \qquad |x| \leq \tfrac{1}{2}a|t|$$

for some C, from which we see that

$$\int_{-\infty}^{\infty} \|F(|x| \leq \tfrac{1}{2}a|t|)e^{-itH_0}(H_0 + i)f\| \, dt < \infty \tag{319}$$

Now write

$$\begin{aligned} Ve^{-itH_0}f = {} & V(H_0+i)^{-1}F(|x| \le \tfrac{1}{2}a|t|)e^{-itH_0}(H_0+i)f \\ & + V(H_0+i)^{-1}F(|x| \ge \tfrac{1}{2}a|t|)e^{iH_0t}(H_0+i)f \end{aligned}$$

Then,

$$\begin{aligned} \|Ve^{-itH_0}f\| \le {} & \|V(H_0+i)^{-1}\| \, \|F(|x| \le \tfrac{1}{2}a|t|)e^{-itH_0}(H_0+i)f\| \\ & + \|V(H_0+i)^{-1}F(|x| \ge \tfrac{1}{2}a|t|)\| \, \|(H_0+i)f\| \end{aligned} \tag{320}$$

By (319) the first term is in $L^1(\mathbb{R}, dt)$. By the Enss condition the second term is in $L^1(\mathbb{R}, dt)$, so

$$\int_{-\infty}^{\infty} \|Ve^{-itH_0}f \, dt\| < \infty.$$

and therefore, by the usual density argument and Cook's method, the wave operators $\Omega^{\pm}(H, H_0)$ exist. In fact, one can say much more. For the two-body case, the basic result is:

Theorem XI.112 (Enss's theorem) Let V be an Enss potential and let $H = H_0 + V$ as a self-adjoint operator sum. Then:

(1) $\Omega^{\pm}(H, H_0)$ exist and are complete.
(2) $\sigma_{\text{sing}}(H)$ is empty.
(3) The only possible (finite) accumulation point for $\sigma_{\text{pp}}(H)$ is 0 and any nonzero eigenvalue has finite multiplicity.

We remark that, in particular, the results of the theorem imply that $\sigma_{\text{ess}}(H) = [0, \infty)$. This conclusion is not automatic from Weyl's theorem (Section XIII.4) since the operator V may not be relatively compact.

The proof of Enss's theorem requires:

Theorem XI.113 Let $H = H_0 + V$ where $H_0 = -\frac{1}{2}\Delta$ and V is an Enss potential. Let φ_n be a sequence of unit vectors so that:

(i) $\lim_{n\to\infty} \|F(|x| \le n)\varphi_n\| = 0$.
(ii) For some $a > 0$, $b > 0$,

$$\lim_{n\to\infty} \|[E_{(-a,a)}(H) + E_{(b,\infty)}(H)]\varphi_n\| = 0$$

where $E_\Omega(H)$ is the family of spectral projections for H.

Then $\varphi_n = \varphi_{n;\,\text{in}} + \varphi_{n;\,\text{out}} + \varphi_{n;\,\text{w}}$ where

$$\overline{\lim}\|\varphi_{n;\,\text{in}}\| < \infty, \qquad \overline{\lim}\|\varphi_{n;\,\text{out}}\| < \infty \tag{321}$$

$$\lim_{n\to\infty} \|(\Omega^+ - 1)\varphi_{n;\,\text{in}}\| = 0 = \lim_{n\to\infty} \|(\Omega^- - 1)\varphi_{n;\,\text{out}}\| \tag{322}$$

$$\lim_{n\to\infty} \sup_{t<0} \|F(|x| \le \delta n)e^{-itH_0}\varphi_{n;\,\text{in}}\| = 0 \tag{323}$$

for some $\delta > 0$, and

$$\lim_{n\to\infty} \|\varphi_{n;\,\text{w}}\| = 0 \tag{324}$$

The basic idea will be to decompose φ_n into pieces, one with momenta pointing outward, the other inward. Along the way we shall have left over pieces which we consign to the wastebasket and lump together as $\varphi_{n;\,\text{w}}$. Of course we could retrieve these pieces from the wastebasket and lump them in with $\varphi_{n;\,\text{in}}$ without affecting (321)–(323), but it is conceptually convenient not to do so. We defer the proof of Theorem XI.113 and first use it to prove Theorem XI.112.

Proof of Theorem XI.112 We have already shown that the wave operators exist. Let $\varphi \in \mathscr{H}_{\text{sing}}(H)$ with $E_{(-a,\,a)}(H)\varphi = E_{(b,\,\infty)}(H)\varphi = 0$ for some a, b. Since $(H_0 + i)(H + i)^{-1}$ is bounded and $F(|x| \le n)(H_0 + i)^{-1}$ is compact, we see that $F(|x| \le n)(H + i)^{-1}$ is compact. Thus, by the RAGE theorem, proven in the appendix, we can pick τ_n inductively so that $\tau_{n+1} > \tau_n > 0$ and $\|F(|x| \le n)e^{-i\tau_n H}\varphi\| \le 1/n$. Let $\varphi_n = e^{-i\tau_n H}\varphi$. Then φ_n obeys the hypotheses of Theorem XI.113 so

$$\|\varphi_n - \Omega^+\varphi_{n;\,\text{in}} - \Omega^-\varphi_{n;\,\text{out}}\| \to 0 \tag{325}$$

Since Ran $\Omega^\pm \subset \mathscr{H}_{\text{ac}}(H) \subset \mathscr{H}_{\text{sing}}^\perp$, and $\mathscr{H}_{\text{sing}}$ is left invariant by e^{-itH}, we see that $\|\varphi_n\| \to 0$, so $\varphi = 0$. It follows that $\mathscr{H}_{\text{sing}}(H) = \{0\}$.

Next let $\varphi \in \mathscr{H}_{\text{ac}}(H)$ and suppose that $\varphi \in (\text{Ran }\Omega^-)^\perp$ and $E_{(-a,\,a)}(H)\varphi = E_{(b,\,\infty)}(H)\varphi = 0$ for some a, b. As above, (325) holds. We have that $(\varphi_n, \Omega^-\varphi_{n;\,\text{out}}) = 0$ since e^{-itH} leaves $(\text{Ran }\Omega^-)^\perp$ invariant. Moreover,

$$\begin{aligned}
|(\varphi_n, \Omega^+\varphi_{n;\,\text{in}})| &= |(\varphi, e^{i\tau_n H}\Omega^+\varphi_{n;\,\text{in}})| \\
&= |((\Omega^+)^*\varphi, e^{i\tau_n H_0}\varphi_{n;\,\text{in}})| \\
&\le \|F(|x| \ge \delta n)(\Omega^+)^*\varphi\|\,\|\varphi_{n;\,\text{in}}\| \\
&\quad + \|\varphi\|\,\|F(|x| \le \delta n)e^{i\tau_n H_0}\varphi_{n;\,\text{in}}\|
\end{aligned}$$

By (321) the first term goes to zero, and by (323) the second does also. Thus, φ_n is asymptotically orthogonal to $\Omega^+\varphi_{n;\,\text{in}} + \Omega^-\varphi_{n;\,\text{out}}$ and so to itself. It follows that $\varphi = 0$, so $(\operatorname{Ran}\Omega^-)^\perp \cap \mathscr{H}_{\text{ac}}(H) = \{0\}$. Thus $\operatorname{Ran}\Omega^- = \mathscr{H}_{\text{ac}}(H)$ and similarly $\operatorname{Ran}\Omega^+ = \mathscr{H}_{\text{ac}}(H)$, so the wave operators are complete.

Finally, suppose that φ_n is a sequence of orthogonal normalized eigenvectors of H, $H\varphi_n = E_n\varphi_n$ and $E_n \to E \neq 0$. If we choose a, b with $E \notin [-a, a] \cup [b, \infty)$, then hypothesis (b) of Theorem XI.113 holds. Moreover, by the compactness of $F(|x| \le R)(H+i)^{-1}$, and the orthonormality of $\{\varphi_n\}$, we have that

$$\|F(|x| \le R)\varphi_n\| = |E_n + i|\;\|F(|x| \le R)(H+i)^{-1}\varphi_n\| \to 0$$

By passing to a subsequence we see that we can suppose that the φ_n obey hypothesis (a) of Theorem XI.113. Thus (325) holds, so that φ_n is asymptotically in $\mathscr{H}_{\text{ac}}(H)$ which is impossible. This contradiction implies that conclusion (3) is valid. ∎

The proof of Theorem XI.113 depends on three preparatory lemmas. The first is an argument that we shall repeat in Section XIII.5 that says that H and H_0 look alike at large distances:

Lemma 1 Let Φ be a continuous function on $\mathbb{R}$ vanishing at infinity. Then

$$\lim_{n\to\infty} \|[\Phi(H) - \Phi(H_0)]F(|x| \ge n)\| = 0 \tag{326}$$

Proof Since H is bounded from below, choose $E_0 < \inf \sigma(H) - 1$. Then, for $z \le E_0 + 1$ and $\Phi(x) = (x-z)^{-1}$, (326) holds since

$$\|[\Phi(H) - \Phi(H_0)]F(|x| \ge n)\| \le \|(H-z)^{-1}\|\;\|V(H_0 - z)^{-1}F(|x| \ge n)\|$$

and the second factor goes to zero by the Enss condition and a simple argument (Problem 151c). Since $(H-z)^{-1} - (H_0 - z)^{-1}$ is uniformly bounded and analytic on $\operatorname{Re} z \le E_0 + 1$, the Vitali convergence theorem implies convergence of derivatives of $[(H-z)^{-1} - (H_0-z)^{-1}]F(|x| \ge n)$ to zero, i.e., (326) holds for $\Phi(x) = (x - E_0)^{-m}$ and thus for Φ a polynomial in $(x - E_0)^{-1}$. But, by the Stone–Weierstrass theorem, such polynomials are $\|\cdot\|_\infty$-dense in the continuous functions on $[E_0 + 1, \infty)$ vanishing at infinity. By an $\varepsilon/3$-argument, (326) results for all claimed Φ. ∎

Secondly, we need a slightly refined version of the Corollary to Theorem XI.14.

Lemma 2 Let K be a compact subset of $\mathbb{R}^\nu$ and let $\mathcal{O}$ be an open neighborhood of K. Let $C(x_0, t) = \{x_0 + vt \mid v \in \mathcal{O}\}$ be the "classically allowed region" for particles starting at x_0 with velocities in $\mathcal{O}$. Then, for any ℓ, there is a number μ and constant D so that

$$|e^{-itH_0}u(x)| \le D(1 + \operatorname{dist}(x, C(x_0, t)))^{-\ell} \|(1 + |x - x_0|^\mu)u\| \tag{327}$$

for all u with supp $\hat{u} \subset K$ and all $x \notin C(x_0, t)$.

Proof Without loss we can suppose that $x_0 = 0$ since e^{-itH_0} commutes with translations. By a limiting argument, we can suppose that $u \in \mathcal{S}$. By Theorem XI.14 and the arguments in the proof of its corollary, for supp $\hat{u} \subset K$, $u \in \mathcal{S}$, and $x \notin C(0, t)$:

$$|(e^{-itH_0}u)(x)| \le D_0(1 + |x| + |t|)^{-\ell} \sum_{|\alpha| \le \ell} \|D^\alpha \hat{u}\|_\infty$$

(327) follows if we note that by a Sobolev estimate and the Plancherel theorem

$$\sum_{|\alpha| \le \ell} \|D^\alpha \hat{u}\|_\infty \le C_0 \sum_{|\alpha| \le \ell + \nu + 1} \|D^\alpha \hat{u}\|_2 \le C_1 \|(1 + |x|^{\ell + \nu + 1})u\|_2$$

and that

$$|\operatorname{dist}(x, C(0, t))| \le C(|x| + |t| + 1) \tag{328}$$

For, let $v_\infty = \sup\{|v| \mid v \in \mathcal{O}\}$. Then, either $|x| \le v_\infty |t|$, in which case $|\operatorname{dist}(x, C(0, t))| \le 2v_\infty |t|$ or $|x| \ge v_\infty |t|$, in which case

$$|\operatorname{dist}(x, C(0, t))| \le 2|x|. \ \blacksquare$$

Finally, we need a lemma about localizations in phase space.

Lemma 3 Let $\mathcal{X}_\alpha$, $\alpha \in \mathbb{Z}^\nu$, be the characteristic function of the unit cube centered at α. Let $f \in \mathcal{S}$ be a fixed positive function and let $f_\alpha \equiv f * \mathcal{X}_\alpha$. Suppose that $\int f\, d^\nu x = 1$. For each $\alpha \in \mathbb{Z}^\nu$, let g_α be a function in $\mathcal{S}$ so that $\sup_\alpha \|(1 - \Delta)^\nu g_\alpha\|_2 < \infty$. Then ($P = -i\nabla$; X = multiplication by x):

(a) $Tu = \sum_\alpha g_\alpha(P) f_\alpha(X)u$ defined a priori on C_0^∞ defines a bounded map from $L^2(\mathbb{R}^\nu)$ to $L^2(\mathbb{R}^\nu)$.

(b) $\|\sum_{|\alpha| \le \frac{3}{4}R} f_\alpha(X)u\|_2 \le C[\|F(|x| \le \frac{7}{8}R)u\|_2 + R^{-1}\|u\|_2]$ for some R-independent constant C.

Proof (a) $\bar{g}_\alpha(P)g_\beta(P)$ is convolution with a function $h_{\alpha\beta}$. We claim that $|h_{\alpha\beta}(x)| \le C_0(1+|x|)^{-2\nu}$ for a constant C_0 independent of α and β. This follows from a uniform bound on $\|\bar{g}_\alpha g_\beta\|_1$ and $\|(-\Delta)^\nu \bar{g}_\alpha g_\beta\|_1$, which by Leibnitz's rule follows from the hypotheses on $\|g_\alpha\|_2$ and $\|(-\Delta)^\nu g_\alpha\|_2$. Thus

$$\begin{aligned}
\|Tu\|^2 &= \sum_{\alpha,\beta} \int \overline{u(x)} f_\alpha(x) h_{\alpha\beta}(x-y) f_\beta(y) u(y)\, dx\, dy \\
&\le C_0 \sum_{\alpha,\beta} \int |u(x)| f_\alpha(x)(1+|x-y|)^{-2\nu} f_\beta(y)|u(y)|\, dx\, dy \\
&= C_0 \int |u(x)|(1+|x-y|)^{-2\nu}|u(y)|\, dx\, dy \\
&\le C_1 \|u\|^2
\end{aligned}$$

where we used $\sum_\alpha f_\alpha = 1$ in the second step and Young's inequality in the last.

(b) Using Young's inequality

$$\|[f * F(|x| \le \tfrac{3}{4}R)]u\| \le \|v\| + \|w\|$$

where

$$\begin{aligned}
\|v\| &= \|[f * F(|x| \le \tfrac{3}{4}R)]F(|x| \le \tfrac{7}{8}R)u\|_2 \\
&\le \|f * F(|x| \le \tfrac{3}{4}R)\|_\infty \|F(|x| \le \tfrac{7}{8}R)u\|_2 \\
&\le \|f\|_1 \|F(|x| \le \tfrac{7}{8}R)u\|_2
\end{aligned}$$

and

$$\begin{aligned}
\|w\| &= \|[f * F(|x| \le \tfrac{3}{4}R)]F(|x| \ge \tfrac{7}{8}R)u\|_2 \\
&\le \|[f * F(|x| \le \tfrac{3}{4}R)]F(|x| \ge \tfrac{7}{8}R)\|_\infty \|u\|_2
\end{aligned}$$

For $|y| \ge \frac{7}{8}R$,

$$\begin{aligned}
(f * F(|x| \le \tfrac{3}{4}R))(y) &= \int_{|x| \le \frac{3}{4}R} f(y-x)\, dy \\
&= \int_{|x| \le \frac{3}{4}R} h(y-x)\, dy
\end{aligned}$$

where $h = fF(|x| \ge \frac{1}{8}R)$, since $y \ge \frac{7}{8}R$ and $|x| \le \frac{3}{4}R$ implies that $|y-x| \ge \frac{1}{8}R$. Thus $\|w\| \le \|F(|x| \ge \frac{1}{8}R)f\|_1 \|u\|_2$. ▮

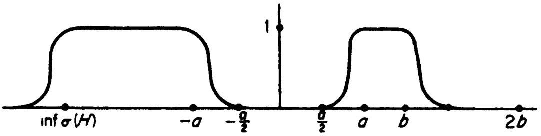


FIGURE XI.16

Proof of Theorem XI.113 Pick a function Φ in $\mathscr{S}(\mathbb{R})$ so that $\Phi = 0$ on $(-\frac{1}{2}a, \frac{1}{2}a)$ and $(2b, \infty)$ and $\Phi = 1$ on $[\inf \sigma(H), -a]$ and $[a, b]$. See Fig. XI.16. Let $\eta_n = \Phi(H_0)\varphi_n$ and

$$\varphi_{n;\,\mathrm{w}}^{(1)} \equiv \varphi_n - \eta_n = [1 - \Phi(H)]\varphi_n + [\Phi(H) - \Phi(H_0)]\varphi_n$$

Then $\|\varphi_{n;\,\mathrm{w}}^{(1)}\| \to 0$ as $n \to \infty$ since the first term goes to zero by hypothesis (ii) of the theorem and the second term goes to zero by hypothesis (i) and Lemma 1. Moreover, since $\Phi(H_0)$ is convolution with a fixed function in $\mathscr{S}$, we have, as in the proof of part (b) of Lemma 3, that

$$\lim_{n \to \infty} \|F(|x| < \tfrac{7}{8}n)\eta_n\| = 0 \tag{329}$$

We now make the promised decomposition into the piece "going out," and that "going in." Let f be a fixed positive function in $\mathscr{S}(\mathbb{R}^\nu)$ so that $\hat{f}$ has support in $\{k \mid |k| < \frac{1}{2}\sqrt{a}\}$ and $\int f(x)\, d^\nu x = 1$. Then $f_\alpha \equiv f * \mathscr{X}_\alpha$ has supp $\hat{f}_\alpha$ also in $\{k \mid |k| < \frac{1}{2}\sqrt{a}\}$ and $\widehat{f_\alpha \eta_n}$ has support in $\{k \mid \frac{1}{2}\sqrt{a} < |k| < 2\sqrt{b} + \frac{1}{2}\sqrt{a}\}$. Fix functions g and h in $\mathscr{S}$ so that: (i) $g(k) + h(k) = 1$ for $|k| < 2\sqrt{b} + \frac{1}{2}\sqrt{a}$; (ii) $g(k) = 0$ (respectively, $h(k) = 0$) if $|k| > \frac{1}{6}\sqrt{a}$ and k makes an angle of less than 30° with the unit vector in the k_1 (respectively, $-k_1$) direction. Let g_α and h_α be the functions obtained by rotating g and h in such a way that the forbidden cone for g_α (respectively, h_α) is about the direction from α back toward 0 (respectively, the negative of this direction), see Fig. XI.17. We

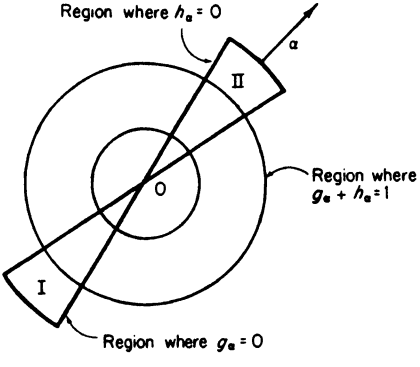

Region where $h_\alpha = 0$
α
II
O
Region where $g_\alpha + h_\alpha = 1$
I
Region where $g_\alpha = 0$

FIGURE XI.17

shall take

$$\varphi_{n;\,\text{in}} = \sum_{|\alpha| \geq \frac{3}{4}n} h_\alpha(P) f_\alpha(X) \eta_n \equiv \sum \eta_{n;\,\alpha,\,\text{in}}$$

$$\varphi_{n;\,\text{out}} = \sum_{|\alpha| \geq \frac{3}{4}n} g_\alpha(P) f_\alpha(X) \eta_n \equiv \sum \eta_{n;\,\alpha,\,\text{out}}$$

$$\varphi_{n;\,\text{w}}^{(2)} = \sum_{|\alpha| \leq \frac{3}{4}n} f_\alpha(X) \eta_n; \qquad \varphi_{n;\,\text{w}} = \varphi_{n;\,\text{w}}^{(1)} + \varphi_{n;\,\text{w}}^{(2)}$$

Since supp $\widehat{f_\alpha \eta_n}$ is contained in the set where $g_\alpha + h_\alpha = 1$, $\varphi_{n;\,\text{in}} + \varphi_{n;\,\text{out}} + \varphi_{n;\,\text{w}}^{(2)} = \eta_n$. Moreover, $\|\varphi_{n;\,\text{w}}^{(2)}\| \to 0$ by part (b) of Lemma 3 and (329). Thus (324) holds, and by part (a) of Lemma 3 so does (321). It remains to show (322) and (323).

We next claim that for some fixed $\delta > 0$, all ℓ, $|\alpha| \geq \frac{3}{4}n$, $t \geq 0$, and $|x| \leq \delta(n + |t|)$,

$$|(e^{-itH_0}(H_0 + i)\eta_{n;\,\alpha;\,\text{out}})(x)| \leq C_\ell(1 + |\alpha| + n + |t|)^{-\ell} \tag{330}$$

Using Lemma 2, this follows from two facts:

(a) $\sup_{n,\alpha} \| |x - \alpha|^\mu (H_0 + i) g_\alpha(P) f_\alpha(x) \eta_n \| < \infty$. This follows from the fact that $\| |x - \alpha|^\mu f_\alpha \|_\infty$ is uniformly bounded and that the derivatives of $(k^2 + i) g_\alpha$ are uniformly bounded.

(b) Let $C_\alpha(t) = \{\alpha + vt \mid v \in \text{supp}\, g_\alpha(k) \cap \{\frac{1}{2}\sqrt{a} \leq |k| \leq 2\sqrt{b} + \frac{1}{2}\sqrt{a}\}\}$. Then for x, α, t as above,

$$\text{dist}(x, C_\alpha(t)) \geq \delta(1 + |\alpha| + n + |t|) \tag{331}$$

so long as δ is sufficiently small. (331) asserts that for $t \geq 0$, $|\alpha| \geq \frac{3}{4}n$, $|x_0| \leq \delta n$, $|w| \leq \delta$, and

$$v \in V_0 \equiv \text{supp}\, g_\alpha \cap \{\tfrac{1}{2}\sqrt{a} < |k| \leq 2\sqrt{b} + \tfrac{1}{2}\sqrt{a}\},$$

we have that $\text{dist}(x_0 + wt, \alpha + vt) \geq c(1 + |\alpha| + n + t)$. Suppose we can show that this distance is always nonzero when α is replaced by $(1 - \varepsilon)\alpha$. Then by shrinking δ we can obtain a lower bound by $2c(1 + |\alpha| + t)$, and using $|\alpha| \geq \frac{3}{4}n$ we obtain the desired estimates. That the distance is nonzero just says that a particle starting at $\alpha - x_0$ with velocity $v - w$ does not hit the origin and this is obvious.

From (330) for exponent $\ell + v/2$, one immediately obtains for $t > 0$ and $|\alpha| \geq \frac{3}{4}n$,

$$\|F(|x| \leq \delta n + a\delta|t|)(H_0 + i)e^{-itH_0}\eta_{n;\,\alpha;\,\text{out}}\| \leq C_\ell'(1 + |\alpha| + n + |t|)^{-\ell}$$

and then that for $t \geq 0$

$$\|F(|x| \leq \delta n + a\delta|t|)(H_0 + i)e^{-itH_0}\varphi_{n;\,\text{out}}\| \leq C_\ell''(1 + n + |t|)^{-2} \tag{332}$$

This, the analogue for $t \leq 0$ with out replaced by in, and (320), imply (322). (323) follows by proving the analogue of (332) without the extra factor of $(H_0 + i)$. ▌

Appendix to XI.17: The RAGE theorem

In this appendix we shall prove a theorem of Wiener on the L^2-mean value of the Fourier transform of a measure and a result of similar genre which we call the RAGE theorem because of contributions made to it by Ruelle, Amrein, Georgescu, and Enss.

Recall that a finite (positive) Baire measure μ on a locally compact space X has $\mu(\{x\}) = 0$ for all but countably many x and that $\sum_{x \in X} \mu(\{x\}) \leq \mu(X) < \infty$ so that $\sum_{x \in X} |(\mu(\{x\})|^2$ is a finite number.

Theorem XI.114 (Wiener's theorem) Let μ be a finite Baire measure on $\mathbb{R}$ and let

$$F(t) = \int e^{-ixt}\, d\mu(x)$$

be its Fourier transform (up to a factor of $(2\pi)^{-1/2}$). Then

$$\lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} |F(t)|^2\, dt = \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2 \tag{333}$$

In particular, if μ has no pure points, then the limit is zero.

Proof Using the formula for F and Fubini's theorem (the measure $d\mu \otimes d\mu \otimes (2T)^{-1}\, dt$ on $\mathbb{R} \times \mathbb{R} \times [-T, T]$ is finite):

$$\frac{1}{2T} \int_{-T}^{T} |F(t)|^2\, dt = \int d\mu(x) \int d\mu(y) \frac{1}{2T} \int_{-T}^{T} e^{-i(x-y)t}\, dt$$

$$= \int d\mu(x) H(T, x)$$

where

$$H(T, x) = \int d\mu(y)[T(x-y)]^{-1} \sin(T(x-y))$$

The integrand in H is pointwise bounded by 1 and converges to 0 (respectively, 1) as $T \to \infty$ if $y \neq x$ (respectively, $y = x$). Using the dominated convergence theorem:

$$\lim_{T \to \infty} H(T, x) = \mu(\{x\}) \qquad \text{and} \qquad |H(T, x)| \leq \mu(\mathbb{R})$$

Using the dominated convergence theorem again,

$$\lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} |F(t)|^2 \, dt = \int d\mu(x) \, \mu(\{x\}) = \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2. \quad \blacksquare$$

We note that this theorem and its proof extend to show that

$$\frac{1}{2N+1} \sum_{n=-N}^{N} |F(n)|^2 \to \sum_{x \in \mathbb{R}} |\mu(\{x\})|^2$$

and that this in turn implies Theorem VII.14b (which we stated without proof in Volume I); see Problem 148.

Definition Let A be a self-adjoint operator. $P_{\text{cont}}(A)$ denotes the projection onto all vectors φ whose spectral measure has no pure points, i.e., $P_{\text{cont}}(A)$ is the projection onto the orthogonal complement of the eigenvectors of A.

Theorem XI.115 (the RAGE theorem) Let A be a self-adjoint operator and let C be a bounded operator, so that $C(A+i)^{-1}$ is compact. Then:

(a) For all $\varphi \in P_{\text{cont}}(A)\mathscr{H}$:

$$\frac{1}{2T} \int_{-T}^{T} \|Ce^{-itA}\varphi\|^2 \, dt \to 0 \tag{334}$$

as $T \to \infty$.

(b) For some $\varepsilon(T) \to 0$ as $T \to \infty$, we have that

$$\frac{1}{2T} \int_{-T}^{T} \|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2 \, dt \leq \varepsilon(T)\|(A+i)\varphi\|^2 \tag{335}$$

for all $\varphi \in D(A)$.

(c) (334) is true if the power 2 is dropped and

$$\frac{1}{2T} \int_{-T}^{T} \|Ce^{-itA}P_{\text{cont}}(A)\varphi\| \, dt \leq \varepsilon(T)^{1/2}\|(A+i)\varphi\| \tag{336}$$

Proof (a) follows by a simple density argument from (b) since $D(A) \cap \operatorname{Ran} P_{\text{cont}}(A)$ is dense in $\operatorname{Ran} P_{\text{cont}}(A)$ and

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}\varphi\|^2\, dt \le \|C\|^2\|\varphi\|^2 \tag{337}$$

(c) follows from (a), (b), and the Schwarz inequality. By writing

$$\|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2 = \|C(A+i)^{-1}e^{-itA}P_{\text{cont}}(A)(A+i)\varphi\|^2,$$

we see that it suffices to prove the analog of (335) where C is compact and $\varepsilon(T)\|(A+i)\varphi\|^2$ is replaced by $\varepsilon(T)\|\varphi\|^2$.

For any C and T, let

$$\varepsilon_C(T) = \sup_{\varphi \ne 0} \|\varphi\|^{-2}(2T)^{-1}\int_{-T}^{T} \|Ce^{-itA}P_{\text{cont}}(A)\varphi\|^2\, dt$$

Then by (337)

$$\varepsilon_C(T) \le \|C\|^2$$

and since $\|a+b\|^2 \le 2\|a\|^2 + 2\|b\|^2$:

$$\varepsilon_{C+D}(T) \le 2\varepsilon_C(T) + 2\varepsilon_D(T)$$

Thus, to show that $\varepsilon_C(T) \to 0$ for compact C, it suffices to prove it for finite rank C and thus for a C of rank 1. Since $P_{\text{cont}}(A)$ commutes with e^{-iAt}, we need only show that for $\psi \in \operatorname{Ran} P_{\text{cont}}(A)$ and all φ:

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt \le \varepsilon(T)\|\varphi\|^2$$

with $\varepsilon(T) \to 0$ as $T \to \infty$.

As in the proof of Lemma 1 before Theorem XI.7, we can pass to a spectral representation, so that

$$(\psi, e^{-itA}\varphi) = \int e^{-itx}h(x)\, d\mu(x)$$

where $d\mu$ is the spectral measure for ψ and $\int |h(x)|^2\, d\mu(x) \le \|\varphi\|^2$. As in the proof of Wiener's theorem:

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt = \int h(x)\, d\mu(x) \int \overline{h(y)}\frac{\sin((x-y)T)}{(x-y)T}\, d\mu(y)$$

Using the Schwarz inequality,

$$\frac{1}{2T}\int_{-T}^{T} |(\psi, e^{-itA}\varphi)|^2\, dt \le \|\varphi\|^2\, \delta(T)$$

with

$$\delta(T) = \left[\int d\mu(x)\, d\mu(y) \left| \frac{\sin((x-y)T)}{(x-y)T} \right|^2 \right]^{1/2}$$

As in the proof of Wiener's theorem, $\delta(T) \to 0$ as $T \to \infty$ since μ has no pure points. ▌

Corollary Let A be a self-adjoint operator on a separable Hilbert space with no point spectrum. Then there exists a sequence $t_n \to \infty$ so that $e^{-it_n A} \to 0$ weakly as $n \to \infty$.

Proof Let $\{\varphi_k\}_{k=1}^{\infty}$ be an orthonormal basis. Then $C = \sum_{k=1}^{\infty} 2^{-k/2}(\varphi_k, \cdot)\varphi_k$ is compact; so by the above proof

$$\frac{1}{2T}\int_{-T}^{T} \|Ce^{-itA}\psi\|^2 \, dt \le \varepsilon(T)\|\psi\|^2$$

with $\varepsilon(T) \to 0$. It follows that

$$\frac{1}{2T}\int_{-T}^{T} \left[\sum_{k,m} 2^{-k-m} |(\varphi_k, e^{-itA}\varphi_m)|^2\right] dt \le \varepsilon(T)$$

Since the function, g, in brackets is positive and goes to zero in mean, there must be a sequence $t_n \to \infty$ so that $g(t_n) \to 0$ (clearly there exists T_n with $\varepsilon(T_n) \le 2^{-n}$ and then $t_n \in (\frac{1}{2}T_n, T_n)$ with $g(t_n) \le 4(2^{-n})$). But if the sum goes to zero, each $(\varphi_k, e^{-it_n A}\varphi_m) \to 0$ as $n \to \infty$, which implies the weak convergence. ▌

If A has continuous singular spectrum, it can happen that e^{-itA} does not go to zero weakly as $t \to \infty$ (Problem 149).

In *our* presentation of the Lax–Phillips theory, we proved a priori the absence of singular continuous spectrum. The RAGE theorem ideas allow one to avoid this (see Problem 150).

We conclude this appendix by giving a result of RAGE type that will probably be useful in the discussion of multiparticle scattering.

Theorem XI.116 Let A be self-adjoint operator with empty singular spectrum. Let C and D be two bounded operators with $(A+i)^{-1}C$ and $D(A+i)^{-1}$ compact. Then for any ε, we can find P, a projection onto a *finite* number of eigenvectors for A and a $T \ge 0$ so that, for $t > T$,

$$\|D(A+i)^{-2}e^{-iAt}(1-P)C\| \le \varepsilon$$

Before proving this theorem, let us describe a special case. Suppose that $C = D = F(|x| \leq n)$ and $A = -\Delta + V$ where V is a local Enss potential. This theorem then says that if φ is initially localized in $|x| \leq n$, i.e., $F(|x| \leq n)\varphi = \varphi$, then φ can be broken into two pieces: $P\varphi + (1 - P)\varphi$. $P\varphi$ is a linear combination of specific bound states. The other piece has the property that if we wait long enough, it will "leave the region" and not return, i.e.,

$$\|F(|x| \leq n)e^{-itH}(1 - P)\varphi\| \leq \varepsilon\|(H + i)^2\varphi\| \qquad \text{for all} \quad t > T_0$$

Proof of Theorem XI.116 As in the proof of the RAGE theorem, we need only find T and P so that, for $t > T$,

$$\|Q_1 e^{-itA}(1 - P)Q_2\| \leq \varepsilon$$

where Q_1 and Q_2 are two rank 1 operators. Let P_{ac} be the projection onto the absolutely continuous space for A, let $\varphi_1, \varphi_2, \ldots$ be a labeling of the eigenvectors for A and let P_n be the orthogonal projection onto the span of the vectors $\varphi_1, \ldots, \varphi_n$. Finally, let $P_\infty = \text{s-lim}\, P_n = 1 - P_{\text{ac}}$. By the Riemann–Lebesgue lemma (see Section IX.2) $\|Q_1 e^{-iAt}P_{\text{ac}} Q_2\| \to 0$ as $t \to \infty$, so we can choose T so that this norm is less than $\varepsilon/2$ for $t > T$. Since Q_2 has rank 1, $\|(P_\infty - P_n)Q_2\| \to 0$ as $n \to \infty$, so that we can choose n with $\|(P_\infty - P_n)Q_2\| \leq (\varepsilon/2)\|Q_1\|$. Choosing $P = P_n$, we have that for $t > T$,

$$\|Q_1 e^{-iAt}(1 - P)Q_2\| \leq \|Q_1 e^{-iAt}P_{\text{ac}}Q_2\| + \|Q_1 e^{-itA}(P_\infty - P_n)Q_2\| \leq \varepsilon \quad \blacksquare$$

NOTES

Section XI.1 The geometric ideas mentioned in the third paragraph of the section determine part of the scattering data without any reference to a comparison dynamics: Basically, scattering cross sections do not require anything more than the geometric ideas while time delay does. For further discussion, see the Davies–Simon paper quoted in the notes to Section 4, J. Dollard, "Scattering into cones, I. Potential scattering," *Comm. Math. Phys.* **12** (1969), 193–203; and J. M. Jauch, R. Lavine, and R. G. Newton, "Scattering into cones," *Helv. Phys. Acta* **45** (1972), 325–330. Various authors have given prescriptions for a quantum-mechanical state to be a "scattering state" or to lie in $\mathscr{H}_{\text{ac}} \oplus \mathscr{H}_{\text{sing}}$ in geometric terms; see D. Ruelle, "A remark on bound states in potential scattering theory," *Nuovo Cimento A* **61** (1969), 655–662; C. Wilcox, "Scattering states and wave operators in the abstract theory of scattering," *J. Functional Analysis* **12** (1973), 257–274; W. Amrein and V. Georgescu, "On the characterization of bound states and scattering states in quantum mechanics," *Helv. Phys. Acta* **46** (1973), 635–658; J. Dollard, "On the definition of scattering subspace in non-relativistic quantum mechanics," *J. Mathematical Phys.* **18** (1977), 229–232 and K. B. Sinha, "On the absolutely and singularly continuous subspaces in scattering theory," *Ann. Inst. H. Poincaré, Sect. A* **26** (1977), 263–277. The ideas of Ruelle are an important ingredient in the work of Enss discussed in Section 17; see that section, its appendix, and its notes.

The S-transformation we have defined, $S = (\Omega^-)^{-1}\Omega^+$, is sometimes called the "EBFM S-matrix" after O. Ekstein, "Theory of time dependent scattering for multichannel processes," *Phys. Rev.* **101** (1956), 880–889; and F. Berezin, L. Faddeev, and R. Minlos, *Proceedings of the Fourth All-Union Mathematical Conference*, Leningrad, 1961. The S'-transformation is called the "Jauch S-matrix" after J. Jauch, "Theory of the scattering operator, I, II," *Helv. Phys. Acta* **31** (1958), 127–158, 661–684. One can express the distinction in quantum scattering by writing two-body scattering in physicists' formal notation. One writes the function $(2\pi)^{-3/2}\psi(\cdot, k)$ of Sections 6 and 7 as $|k, \text{in}\rangle$ and the analogous state, $(2\pi)^{-3/2}\psi(\cdot, -k)$, which describes a state that is asymptotically a plane wave in the future as $|k, \text{out}\rangle$. Finally, write $(2\pi)^{-3/2}e^{ik\cdot x}$ as $|k, \text{free}\rangle$. The quantity of physical interest is $S(k, k') = \langle k, \text{out}\,|\,k', \text{in}\rangle$. S and S' are formally given by

$$\begin{aligned} S(k, k') &= \langle k, \text{free}\,|\,S\,|\,k', \text{free}\rangle \\ &= \langle k, \text{in}\,|\,S'\,|\,k', \text{in}\rangle \end{aligned}$$

We see explicitly that S and S' are related by the similarity transformation $\Omega^+\colon |k, \text{free}\rangle \mapsto |k, \text{in}\rangle$.

Section XI.2 Much of this section and, in particular, Theorems XI.1, XI.2, and XI.3, are from B. Simon, "Wave operators for classical particle scattering," *Comm. Math. Phys.* **23** (1971), 37–48. Similar results in a different framework have been found by J. Cook, "Banach algebras and asymptotic mechanics," in *Cargese Lectures in Theoretical Physics* (F. Lurchit, ed.) Gordon and Breach, New York, 1967; by W. Hunziker, "The S-matrix in classical mechanics," *Comm. Math. Phys.* **8** (1968), 282–299; and by R. Prosser, "On the asymptotic behavior of certain dynamical systems," *J. Mathematical Phys.* **13** (1972), 186–196. Cook, Hunziker, and Prosser work in the framework of $L^2(\Sigma, d^6x)$ and define unitary operators by $(U_t^{(0)}f)(w) = f(T_t^{(0)}w)$ and $(U_t f)(w) = f(T_t w)$. They then form wave operators as $\text{s-lim}_{t\to\pm\infty} U_{-t}U_t^{(0)}$ using the methods developed in quantum theory. We feel that the treatment directly on phase space is more natural.

The beautiful argument used in Theorem XI.3 to prove that $\mu(N_+ \Delta N_-) = 0$ appeared in J. E. Littlewood, "On the problem of n bodies," *Comm. Sem. Math. Lund*, tome supp. dédié à M. Riesz (1952), 143–151, and C. L. Seigel, *Vorlesungen über Himmelsmechanik*, Springer-Verlag, New York, Heidelberg, Berlin, 1956; it was rediscovered by Hunziker in the reference quoted above. Littlewood also considered some cases with Coulomb forces.

Scattering from central potentials, that is, the formula (7), is discussed and derived in a variety of textbooks; see, for example, L. Landau and E. Lifshitz, *Classical Mechanics*, Pergamon Press, New York, 1960; or R. Newton, *Scattering Theory of Waves and Particles*, McGraw-Hill, New York, 1966.

The use in Theorem XI.3 of the formula $\dot{I} = \dot{\mathbf{r}}^2 + \mathbf{r}\cdot\mathbf{F}$ is closely connected to the virial theorem (see Landau–Lifshitz). In the central case, its use can be replaced with an application of conservation of energy and of angular momentum (see Problem 14).

Section XI.3 Many of the notions of the abstract time-dependent theory were developed first in the context of two-body quantum systems as described in Section 4. Wave operators were first formalized by C. Møller in "General properties of the characteristic matrix in the theory of elementary particles," I, *Danske. Vid. Selsk. Mat.-Fys. Medd.* **23** (1945), 1–48, who was not precise about what notion of limit was to be used. K. Friedrichs in "On the perturbation of continuous spectra," *Comm. Pure Appl. Math.* **1** (1948), 361–406, introduced wave operators in a class of models where V is rank one. This paper of Friedrichs also contained ideas germinal to the perturbation theory of embedded eigenvalues as described in Sections XII.5 and XII.6. Friedrich's work remained dormant until the work of Jauch (quoted in the Notes to Section 1), Cook, and Kato (quoted below) in 1957–1958.

Cook's method (Theorem XI.4) appeared in J. Cook, "Convergence of the Moller wave matrix," *J. Math. and Phys.* **36** (1957), 82–87, in the concrete situation, $\mathscr{H} = L^2(\mathbb{R}^3)$, $V \in L^2$, $A = -\Delta + V$; $B = -\Delta$. Theorem XI.5 is an abstraction of the idea of J. Kupsch and W. Sandhas, "Møller operators for scattering on singular potentials," *Comm. Math. Phys.* **2** (1966), 147–154. Until recently, the only way known to treat wave operators when $A - B$ is given as a quadratic form was to rely on more sophisticated and complicated methods than Cook's such as the Kato–Birman theory. A theorem stronger than Theorem XI.6 was proven by M. Schechter, "A new criterion for scattering theory," *Duke Math. J*, **44** (1977), 863–877, who relied on time-independent methods rather than Cook's method. Motivated by Schechter's work, B. Simon in "Scattering theory and quadratic forms: On a theorem of Schechter," *Comm. Math. Phys.* **53** (1977), 151–153, proved Theorem XI.6 as we prove it in the text. This theorem has been extended to the case of two Hilbert space scattering by Schechter in "Wave operators for pairs of spaces and the Klein–Gordon equation," *Aequationes Mathematicae*, to appear.

The Kato–Birman theory has as one of its consequences an invariance theorem for the absolutely continuous spectrum with a hypothesis on the perturbation that is independent of the perturbed operator. A similar kind of theorem exists for the essential spectrum; see Section XIII.4. Unfortunately, no such invariance theorem can exist for the singular continuous spectrum. For it is possible to find a self-adjoint operator A and a rank one perturbation C so that A has no singular continuous spectrum but $A + C$ does. This example is discussed in Section XIII.6. As a result, any invariance theorem for the singular continuous spectrum must make hypotheses that relate the perturbation and the unperturbed operator.

What we have chosen to call the Kato–Birman theory has an involved history. Kato introduced the notion of generalized wave operators and proved that $\Omega^{\pm}(A, B)$ exist and are complete if $A - B$ is finite rank in "On finite dimensional perturbations of self-adjoint operators," *J. Math. Soc. Japan* **9** (1957), 239–249. This was extended to the case $A - B \in \mathscr{I}_1$ with A and B purely absolutely continuous in M. Rosenblum, "Perturbations of continuous spectrum and unitary equivalence," *Pacific J. Math.* **7** (1957), 997–1010; and then to the general trace class case (Theorem XI.8) in T. Kato, "Perturbation of continuous spectra by trace class operators," *Proc. Japan Acad.* **33** (1957), 260–264. These results were proven by basically time-independent methods; a fully time-dependent proof was given by Kato in his book *Perturbation Theory For Linear Operators*, Springer-Verlag, New York, Heidelberg, Berlin, 1966.

The idea of using resolvents to extend the Kato–Rosenblum theorem to cases where $A - B$ is unbounded is due to R. Putnam, "Continuous spectra and unitary equivalence," *Pacific J. Math.* **7** (1957), 993–995. S. Kuroda, in "Perturbations of continuous spectra by unbounded operators, I, II," *J. Math. Soc. Japan* **11** (1959), 247–262; **12** (1960), 243–257, proved a weak version of Theorem XI.9, namely, if $B - A$ is relatively B-bounded and $(A + i)^{-1} = (B + i)^{-1} + (A + i)^{-1}C^*D(B + i)^{-1}$ with both $C(B + i)^{-1}$ and $D(A + i)^{-1}$ Hilbert–Schmidt, then $\Omega^{\pm}(A, B)$ exist and are complete. Theorem XI.9 in case A and B are bounded from below is due to M. Birman, "Conditions for the existence of wave operators," *Dokl. Akad. Nauk SSSR* **143** (1962), 506–509. The general case is due to L. deBranges, "Perturbation of self-adjoint transformations," *Amer. J. Math.* **84** (1962), 543–580; and M. Birman, "A criterion for existence of wave operators," *Izv. Akad. Nauk. SSSR Ser. Mat.* **27** (1963), 883–906.

Theorem XI.10 is due to M. Birman, "A local criterion for the existence of wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **32** (1968), 914–942, (English translation: *Math. USSR-Izv.* **2** (1968), 879–906), whose proof is generally regarded as quite difficult.

The original proofs of the Kato–Birman theory were quite a bit more complicated than the one presented in our proof of Theorem XI.7. The basic idea of that proof was hinted at in D. B. Pearson, "General theory of potential scattering with absorption at local singularities," *Helv. Phys. Acta* **47** (1974), 249–264; and, following suggestions by J. Ginibre and T. Kato, presented in D. B. Pearson, "A generalization of Birman's trace theorem," *J. Functional Anal.* **28** (1978), 182–186. Pearson stated the theorem with the extra factor of J—earlier proofs could also extend this way—which led to the unified approach which we present. The proof we give of Theorem XI.9 and the proof in Problem 25 appear to be new. The proof of Theorem XI.10 from this point of view is due to J. Ginibre and D. Pearson and the proof of Theorem XI.13 from this point of view is due to P. Deift, *Classical Scattering Theory with a Trace Condition*, Princeton Series in Physics, Princeton Univ. Press, to appear. The reference for Theorem XI.13 is given in the Notes to Section 10. Theorem XI.12 is due to D. Yafeev, "A remark concerning the theory of scattering for a perturbed polyharmonic operator," *Math. Notes* **15** (1974), 260–265. We follow the proof given by Reed and Simon who rediscovered Yafeev's result in their paper quoted in the notes to Section 10. The part of the conclusion of Theorem XI.12 involving $\Omega^{\pm}(A, B)$ follows directly from Birman's theorem.

The Kato–Birman theory has been extended to certain pairs $\langle A, B\rangle$ where A is self-adjoint but V is only assumed to be such that iB is maximal accretive by E. B. Davies in *Two Channel Hamiltonians and the Optical Model of Nuclear Scattering*, Oxford Univ. Press, preprint, 1978.

The invariance principle, Theorem XI.11, was proven in successively more complicated situations by Birman in the 1962 and 1963 papers quoted above and T. Kato, "Wave operators and unitary equivalence," *Pacific J. Math.* **15** (1965), 171–180.

The general invariance principle (Theorem XI.23) is due to C. Chandler and A. Gibson, "Invariance principle for scattering with long-range (and other) potentials," *Indiana Univ. Math. J.* **25** (1976), 443–460, whose proof we follow. Earlier results were somewhat weaker in that they required $|t|^{\alpha}\|w'(t)\|_2 \in L^1$ for some $\alpha > \frac{1}{2}$ or at least that $\|w(t) - \Omega^{\pm}u\| = O(t^{-1/2})$ as $t \to \mp\infty$. This is not strictly weaker, but is weaker in most practical situations. The early results appeared in L. A. Sakanovich, "The invariance principle for generalized wave operators," *Functional Anal. Appl.* **5** (1971), 49–55; V. B. Matveev, "The invariance principle for generalized wave operators," *Topics Math. Phys.* **5** (1972), 77–85; and *Theoret. and Math. Phys.* **8** (1971), 663–667; and J. A. Donaldson, A. G. Gibson, and R. Hirsh, "On the invariance principle of scattering theory," *J. Functional Analysis* **14** (1973), 131–145. The result of Chandler and Gibson is stated for a slightly larger class of φ's and is applicable to wave operators with modifications for long-range potentials (see Section 9) and for the two Hilbert space theory.

Other general results on invariance of wave operators have been obtained by M. Wollenberg, "The invariance principle for wave operators," *Pacific J. Math.* **59** (1975), 303, and by P. Obermann and M. Wollenberg, "Abel Wave Operators, I: General theory," *Math. Nachr.* (to appear), and "II: Wave operators for functions of operators," *J. Functional Analysis* (to appear). In the latter papers it is shown that if a weaker notion of wave operator is used, the invariance principle *always* holds.

It is not true, in general, that if $\varphi(A) - \varphi(B)$ is trace class, then $\Omega^{\pm}(A, B)$ exist. For example, take $\varphi(x) = x^2$ and A = multiplication by x, B = multiplication by $|x|$ on $L^2(\mathbb{R})$. However, if φ is invertible, this is certainly true and more generally if for each r, there is an admissible function φ_r with $\varphi_r(A) - \varphi_r(B)$ trace class and φ_r one-to-one on $(-r, r)$, then $\Omega^{\pm}(A, B)$ exist and are complete. This result is discussed in the Kato and Deift books quoted above. As a typical application, one has the following proof of Theorem XI.9: $(A+i)^{-1}-(B+i)^{-1}$ in $\mathscr{I}_1$ implies that $(A+ir)^{-1}-(B+ir)^{-1}$ is in $\mathscr{I}_1$ for all $r \neq 0$, which implies that its real part $\varphi_r(A)-\varphi_r(B)$ is in $\mathscr{I}_1$ where $\varphi_r(x) = \mathrm{Re}(x+ir)^{-1} = x(x^2+r^2)^{-1}$. This φ_r obeys the hypothesis of the theorem above, so $\Omega^{\pm}(A, B)$ exist and are complete.

Theorem XI.8 fails in a strong way when $A - B$ is only Hilbert–Schmidt for J. von Neumann, in "Charakterisierung des Spectrums eines Integral-Operators," *Actualités Sci. Indust.* **229** (1935), 38–55, proved that, given any self-adjoint B, there is an A with pure point spectrum and $A - B$ Hilbert–Schmidt. This was extended to the trace ideals $\mathscr{I}_p$ with $p > 1$ in S. Kuroda, "On a theorem of Weyl–von Neumann," *Proc. Japan Acad.* **34** (1958), 11–15.

The Kato–Birman theory has been applied to a variety of situations not discussed in the later sections of the book: There are applications to the spectrum of Toeplitz operators in M. Rosenblum, "The absolute continuity of Toeplitz's matrices," *Pacific J. Math.* **10** (1960), 987–996; and to neutron scattering in Y. Shizuta, "On the fundamental equations of spatially independent problems of neutron thermalization theory," *Progr. Theoret. Phys.* **32** (1964), 489–511.

We describe the history of the two Hilbert space scattering theory in more detail in the notes to Section 10. We mention that the kinematics (Propositions 4 and 5) was systematically developed in T. Kato, "Scattering theory with two Hilbert spaces," *J. Functional Analysis* **1** (1967), 342–369, and that Theorem XI.13 is due to A. Belopol'skii and M. Birman, "The existence of wave operators in scattering theory for pairs of spaces," *Izv. Akad. Nauk SSSR Ser. Mat.* 32 (1968) (English translation: *Math. USSR-Izv.* 2 (1968), 1117–1130).

The idea that stationary phase methods are relevant to scattering theory goes back at least to W. Brenig and R. Haag, "General quantum theory of collision processes," *Fortschr. Physik* **7** (1959), 183–242 (English translation: in *Quantum Scattering Theory* (M. Ross, ed.), Indiana Univ. Press, Bloomington, Indiana, 1963). It is used in various works on long-range scattering; see, for example, the paper of Buslaev and Matveev quoted in the Notes to Section 9, and was raised to a high art by L. Hörmander in his paper quoted in the Notes to Section 9. We follow his presentation closely in Theorems XI.14, XI.15, and XI.16. Theorem XI.17 is important in the Haag–Ruelle scattering theory; we describe its history in the Notes to Section 16.

Theorem XI.20 appears in E. Seiler and B. Simon, "Bounds in the Yukawa$_2$ quantum field theory: Upper bound on the pressure, Hamiltonian bound and linear lower bound," *Comm. Math. Phys.* **45** (1975), 99–114. Theorems asserting that $f(X)g(-i\nabla)$ is trace class for suitable f, g go back to W. Stinespring, "A sufficient condition for an integral operator to have a trace," *J. Reine Angew. Math.* **200** (1958), 200–207, whose results allow f to be of the form given in Theorem XI.21 but restrict g severely. Theorem XI.21 is a special case of a result of M. S. Birman and M. Z. Solomjak, "On estimates of singular numbers of integral operators, III," *Vestnik Leningrad Univ. Fiz. Him.* **24** (1969) (Amer. Math. Soc. *Transl.* **2** (1975)). They introduce the norm

$$\|f\|_{\mathrm{BS}} = \sum_{m \in Z^n} \left(\int_{0 \le x_i \le 1} |f(x-m)|^2 \, dx \right)^{1/2}$$

and show that if $\|f\|_{\mathrm{BS}}$ is finite and $g \in L^2_\delta$, then $f(x)g(-i\nabla)$ is trace class. Since it is easy to show that $\|f\|_{\mathrm{BS}} \le C\|f\|_{L_\delta^2}$, their result implies Theorem XI.21. One can actually show (Problem 37) that it suffices that $\|f\|_{\mathrm{BS}}$ and $\|g\|_{\mathrm{BS}}$ be finite. Conversely, if f and g are nonzero, this condition is also necessary; see B. Simon's book "Trace Ideal Methods," London Math. Soc. Lecture Notes, Cambridge Univ. Press, London and New York, 1979. T. Kato has independently proven Theorems XI.20 and XI.21 (unpublished). We follow Kato's proof of Theorem XI.21. Theorem XI.22 is due to M. Cwikel, "Weak type estimates for singular values and the number of bound states of Schrödinger operators," *Ann. of Math.* **106** (1977), 93–102. Earlier B. Simon, "Analysis with weak trace ideals and the number of bound states of Schrödinger operators," *Trans. Amer. Math. Soc.* **224** (1977), 367–380, had proven the result under the stronger hypotheses $\check{g} \in L^{q'}_{w}(\mathbb{R}^n)$, $q' = q/(q-1)$, and $f \in L^{q-\varepsilon} \cap L^{q-\varepsilon}$ for some $\varepsilon > 0$. There is a theorem of the genre of Theorem XI.22 for the case $1 < q < 2$ using norms related to the $\|\cdot\|_{\mathrm{BS}}$ norm; see Simon's book.

The relation $H_{\mathrm{D}}^2 - m^2 = 2m(1 \otimes H_{\mathrm{S}})$ used in the discussion of Example 2 in the third appendix goes back at least as far as M. H. Johnson and B. A. Lippman, "Motion in a constant magnetic field," *Phys. Rev.* **76** (1949), 828–832. The corresponding invariance of scattering is "obvious" to the physicist who thinks in time-independent terms; see the remarks on the invariance principle in the third appendix to Section 8. At first sight it may appear surprising that one can prove that $\Omega^{\pm}(H_{\mathrm{S}}(A), H_{\mathrm{S}}(0))$ exist without any hypotheses on B, using only hypotheses on A. Notice that $B = \operatorname{curl} A$ can have less falloff at infinity than A if A oscillates rapidly, so that the aforementioned phenomenon is connected with the ideas of Appendix 2 to Section 8 and the references in the notes to that section. In fact, it should be possible to prove many of the results of Combescure–Ginibre and Schechter quoted in those notes by using the identity $H_{\mathrm{D}}^2 - m^2 = 2m(1 \otimes H_{\mathrm{S}})$.

Section XI.4 Theorem XI.24 was first proven in case $V \in L^2$ by J. Cook in his basic paper quoted in the Notes to the preceding section. The extension to potentials with $|x|^{-1-\varepsilon}$ falloff is due to M. Hack, "On the convergence to the Møller wave operators," *Nuovo Cimento* **9** (1958), 731–733. About the same time, S. Kuroda, "On the existence and the unitarity property of the scattering operator," *Nuovo Cimento* **12** (1959), 431–454, proved a similar result. Extensions to n dimensions are discussed in F. Brownell, "A note on Cook's wave matrix theorem," *Pacific J. Math* **12** (1962), 47–52. For central potentials, an improved result can be found in E. Lundquist, "On the existence of the scattering operator," *Ark. Mat.* **7** (1967), 145–157. Lundquist's results are implied by Theorem XI.31, but he only uses Cook's method. Extensions of Cook's method to include magnetic fields can be found in T. Ikebe and T. Tayoshi, "Wave and scattering operators for second order elliptic operators in $\mathbb{R}^3$," *Publ. Res. Inst. Math. Sci.* Kyoto **A4** (1968), 483–496.

Extensions of the Hack–Cook theorem to study $-\Delta + V$ where V is not necessarily a multiplication operator can be found in K. Jörgens and J. Weidmann, "Zur Existenz der Wellenoperatoren," *Math. Z.* **131** (1973), 141–151; K. Veselić and J. Weidmann, "Existenz der Wellenoperatoren fur eine allgemeine Klasse von Operatoren," *Math. Z.* **134** (1973), 255–274; "Asymptotic estimates of wave functions and the existence of wave operators," *J. Functional Analysis* **17** (1974), 61–77; C. Wilcox, "Scattering states and wave operators in the abstract theory of scattering," *J. Functional Analysis* **12** (1973), 257–274; and A. M. Berthier and P. Collet, "Existence and completeness of the wave operators in scattering theory with momentum dependent potentials," *J. Functional Analysis* **26** (1977), 1–15.

Theorem XI.25 is due to Kupsch and Sandhas in their paper and Theorem XI.26 is essentially in the Schechter paper, both quoted in the Notes to Section 3. Theorem XI.27 is due to J. Avron and I. Herbst, "Spectral and scattering theory of Schrödinger operators related to the Stark effect," *Comm. Math. Phys.* **52** (1977), 239–254. Further discussion of Theorem XI.25 can be found in D. Robinson, "Scattering theory with singular potentials I. The two-body problem," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 185–216. Theorems of the type of Theorem XI.30 for $n \leq 3$ appeared first in Kuroda's paper quoted above. Theorem XI.31 is due to S. Kuroda, "On a theorem of Green and Lanford," *J. Mathematical Phys.* **3** (1962), 933–935.

The relation $\overline{S\psi(x)} = (S^*\bar{\psi})(x)$ is called "time reversal invariance" because of a fundamental symmetry of the Hamiltonians, which we discuss. Denote the map $\psi \mapsto \bar{\psi}$ by T. T is antilinear and $TH_0 = H_0 T$, $TV = VT$. Thus $Te^{iH_0 t} = e^{-iH_0 t}T$ and $Te^{iHt} = e^{-iHt}T$. Because of this change of sign, T is called time reversal. One sees immediately that $T\Omega^\pm = \Omega^\mp T$ so that $T(\Omega^-)^*\Omega^+ = (\Omega^+)^*\Omega^- T = [(\Omega^-)^*\Omega^+]^*T$ from which $\overline{S\psi} = S^*\bar{\psi}$ follows. For particles with spin, time reversal is more complicated. The use of time reversal in quantum theory was first emphasized by E. P. Wigner in "Uber die Operation der Zeitumkehr in der Quantenmechanik," *Nachr. Akad. Wiss. Gottingen Math.-Phys. Kl. II* (1931), 546–559.

Theorems of the genre of Theorem XI.32 are due to P. Deift and B. Simon, "On the decoupling of finite singularities from the question of asymptotic completeness in two-body quantum systems," *J. Functional Analysis* **23** (1976), 218–238. Deift and Simon relied on decoupling with Dirichlet boundary conditions (see Section XIII.15) and Feynman path integral estimates. Their results were considerably generalized and extended by M. Combescure and J. Ginibre, "Scattering and local absorption for the Schrödinger operator," *J. Functional Analysis* **29** (1978), 54–73, who used a smooth cutoff J as in the proof we give. Our proof is patterned on theirs. Both papers were motivated by attempts to understand Pearson's example. Pearson's counterexample appeared in D. Pearson, "An example in potential scattering illustrating the breakdown of asymptotic completeness," *Comm. Math. Phys.* **40** (1975), 125–146, where the details of the counterexample may be found. Earlier than Pearson's paper, several examples where $\text{Ran}\,\Omega^+ \neq \text{Ran}\,\Omega^-$ existed, but they all involved pathological behavior at ∞; see T. Kato and S. Kuroda, "A remark on the unitarity property of the scattering operator," *Nuovo Cimento* **14** (1959), 1102–1107; and "The abstract theory of scattering," *Rocky Mountain J. Math.* **1** (1971), 127–171.

References for cluster properties appear in the Notes to the next section.

There is an extensive literature on scattering theory for time-dependent potentials: E. Davies, "Time-dependent scattering theory," *Math. Ann.* **210** (1974), 149–162; J. Goldstein, "Temporally inhomogeneous scattering theory," in *Analyse fonctionnelle et applications* (L. Nachbin, ed.), pp. 125–132, Hermann, Paris, 1975; J. Goldstein and C. Monlezun, "Temporally inhomogeneous scattering theory, II; approximation theory and second order equations," *SIAM J. Math. Anal.* **7** (1976), 276–290; J. Hendrickson, "Temporally inhomogeneous scattering theory for modified wave operators," *J. Mathematical Phys.* **16** (1975), 768–771; and "N-body scattering into cones with long-range time-dependent potentials," *J. Mathematical Phys.* **17** (1976), 729–733; J. Howland, "Stationary scattering theory for time-dependent Hamiltonians," *Math. Ann.* **207** (1974), 315–335; A. Inoue, "An example of temporally inhomogeneous scattering," *Proc. Japan Acad.* **49** (1973), 407–410; and "Wave and scattering operators for an evolving system $d/dt - iA(t)$," *J. Math. Soc. Japan* **26** (1974), 608–624; C. Monlezun, "Temporally inhomogeneous scattering theory," *J. Math. Anal. Appl.* **47** (1974), 133–152; E. Schmidt, "On scattering by time-dependent perturbations," *Indiana Univ. Math. J.* **24** (1975), 925–935; K. Yajima, "Scattering theory for Schrödinger equations with potentials periodic in time;" *J. Math. Soc. Japan* **29**, (4), to appear; S. T. Kuroda and H. Morita, "An estimate for solutions of Schrödinger equations with time-dependent potentials and the associated scattering theory," *J. Fac. Sci. Tokyo* **24** (1977), 459–475; and J. Howland, "Scattering theory for Hamiltonians periodic in time," *Indiana Univ. Math. J.* to appear.

Example 3 is discussed in E. B. Davies, "Scattering from infinite sheets," *Proc. Cambridge Philos. Soc.* (to appear) where the details of the argument that $\text{Ran}\,\Omega^+ = \text{Ran}\,\Omega^-$ can be found. Davies also proves a result of interest for the physical interpretation of the approximation by scattering from a single site. Explicitly, if $|W(x)| \le C(1 + |x|)^{-\alpha}$ and

$$V_L(x) = \sum_{n_2, n_3 \in \mathbb{Z}} W(x_1, x_2 - n_2 L, x_3 - n_3 L)$$

then the wave operators $\Omega^{\pm}(-\Delta + V_L, -\Delta)$ converge strongly to $\Omega^{\pm}(-\Delta + W, -\Delta)$ as $L \to \infty$. This result follows from a general convergence theorem (Problem 16).

Example 4 is discussed in E. B. Davies and B. Simon, "Scattering theory for systems with different spatial asymptotics on the left and right," *Comm. Math. Phys.* (to appear). Earlier references for scattering involving potentials $V(x)$ with limits as $x \to +\infty$ or as $x \to -\infty$ but distinct limits include P. Alsholm and T. Kato, "Scattering theory with long range potentials," *Proc. Amer. Math. Soc. Institute on Partial Differential Equations, 1971*, pp. 393–399 (see Remark (4) on p. 394) and S. Ruijsenaars and P. Bongaarts, "Scattering theory for one-dimensional step potentials," *Ann. Inst. H. Poincaré Sect. A* **26** (1977), 1–17. See Section 17 for another approach to completeness in two-body systems.

Section XI.5 For additional discussion of N-body quantum systems, see Sections XI.17, XIII.2, XIII.3, XIII.5, XIII.10, XIII.11, and XIII.13. A brief readable account of many of the elements of the theory and especially of scattering theory may be found in W. Hunziker, *Mathematical Theory of Multi-particle Quantum Systems*, Lectures in Theoretical Physics, Vol. X (A. Barut and W. Britten, eds.); Gordon and Breach, New York, 1968.

Formal elements of N-body scattering from a wave operator point of view and especially channel orthogonality were first discussed by Jauch in the second paper in his series quoted in the notes to Section 1. Hack's theorem (Theorem XI.34) appeared in "Wave operators in multichannel scattering," *Nuovo Cimento Ser. X* **13** (1959), 231–236. An extension of Hack's theorem to potentials with certain local singularities (essentially an n-body analogue of Theorem XI.25) is proven in W. Hunziker, "Time-dependent scattering theory for singular potentials," *Helv. Phys. Acta* **40** (1967), 1052–1062. See also P. Ferrerro, O. de Pazzis, and D. Robinson, "Scattering theory with singular potentials, II. The N-body problem and hard cores," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 217–232.

The most comprehensive N-body completeness results have been proven, thus far, in case $N = 3$. The basic idea and techniques as well as the earliest results are due to L. Faddeev, *Mathematical Aspects of the Three Body Problem in Quantum Scattering Theory*, Israel Program for Scientific Translation, 1965 (original Russian monograph published by Steklov Institute, 1963). Important technical improvements and extensions of his results are due to L. Thomas, "Asymptotic completeness in two and three particle quantum mechanical scattering," *Ann. Physics* **90** (1975), 127–165; and J. Ginibre and M. Moulin, "Hilbert space approach to the quantum mechanical three body problem," *Ann. Inst. H. Poincaré Sect. A* **21** (1974), 97–145. In particular, Theorem XI.37 is proven in the Ginibre-Moulin paper.

There have been a number of attempts to extend Faddeev's program to N bodies. Analogues of his basic integral equations are due to O. A. Yakubovsky, "On the integral equations in the theory of N-particle scattering," *Soviet J. Nuclear Phys.* **5** (1967), 937–942; and E. Berezin, "Asymptotic behavior of eigenfunctions of Schrödinger's equation for many particles," *Dokl. Akad. Nauk SSSR* (1965) (English translation: *Soviet Math. Dokl.* **6** (1965), 997–1001). Parts of the analysis have been extended by K. Hepp (using Yakubovsky's equations) in "On the quantum mechanical N-body problem," *Helv. Phys. Acta* **42** (1969), 425–458; and by I. Sigal (using Berezin's equations) in "Asymptotic completeness of multiparticle systems," *Dokl. Akad. Nauk SSSR* **204** (1972) (English translation: *Soviet Math. Dokl.* **13** (1972), 756–760). Both analyses are incomplete in that it is required that certain integral equations in certain auxiliary Banach spaces do not have solutions. Faddeev was able to solve this problem and thus finish the analysis in case $N = 3$ by appealing to results on two-body systems. An abstract version of the Faddeev program in the language of the Kato–Kuroda theory of eigenfunction expansions (see the Notes to Section 6) appears in J. Howland, "Abstract stationary theory of multichannel scattering," *J. Functional Anal.* **22** (1976), 250–282.

Asymptotic completeness for certain special multichannel systems with more than three particles has been announced by G. Hagedorn, "Asymptotic completeness for a class of four particle Schrödinger operators," *Bull. Amer. Math. Soc.* **84** (1978), 155–156, and I. Sigal, "On quantum mechanics of many-body systems with dilation analytic potentials," *Bull. Amer. Math. Soc.* **84** (1978), 152–154.

A different approach from Faddeev's has been advocated by P. Deift and B. Simon in "A time dependent approach to the completeness of multiparticle quantum systems," *Comm. Pure Appl. Math.* **30** (1977), 573–583. They prove a kind of analogue to Proposition 3 in Section 3.

Cluster properties of multichannel wave operators and scattering operators were first derived in W. Hunziker, "Cluster properties of multiparticle systems," *J. Mathematical Phys.* **6** (1965), 6–10. Similar cluster properties under time translations are proven in J. R. Taylor, "Timelike cluster properties in nonrelativistic scattering," *J. Mathematical Phys.* **8** (1967), 2131–2137. The study of these properties was motivated by a discussion of cluster properties to be expected for relativistic *S* operators in E. H. Wichmann and J. H. Crichton, "Cluster decomposition properties of the *S*-matrix," *Phys. Rev.* **132** (1963), 2788–2799. Cluster properties for the *S*-matrix derived from a quantum field theory obeying the Wightman axioms and possessing a mass gap are proven in K. Hepp, "Spatial cluster decomposition properties of the *S*-matrix," *Helv. Phys. Acta* **37** (1964), 659–662 and "One-particle singularities of the *S*-matrix in quantum field theory," *J. Mathematical Phys.* **6** (1965), 1762–1767. One important consequence of the cluster properties is that a complete knowledge of the scattering states of charge zero determines the scattering of charged particles. For example, one could study electron–electron scattering by considering states with two electrons and two positrons far away. As the positrons are taken to infinity, the cluster property tells us that the electron–electron scattering amplitude will be recovered in the limit.

The Kato–Birman theory has been applied to prove completeness of *n*-body scattering in the energy range where the system cannot break up into three or more clusters. This result is due to J. M. Combes, "Time dependent approach to nonrelativistic multichannel scattering," *Nuovo Cimento A* **64** (1969), 111–144; see also B. Simon, "Geometric methods in multiparticle quantum systems," *Comm. Math. Phys.* **55** (1977), 259–274, and "*N*-Body scattering in the two-cluster region," *Comm. Math. Phys.* **58** (1978), 205–210.

References for further study of analytic properties of the scattering amplitude in the two-body case appear in the Notes to Section 7. Analytic properties in the *N*-body case are partially treated in the work of Faddeev and Hepp quoted above and more fully in P. Federbush, "Results on the analyticity of many-body scattering amplitudes in perturbation theory," *J. Mathematical Phys.* **8** (1967), 2415–2419; M. Rubin, R. Sugar, and G. Tiktopolous, "Dispersion relations for 3 particle scattering amplitudes, I, II," *Phys. Rev.* **146** (1966), 1130–1149; **159** (1967), 1348–1362; and F. Riahi, "On the analyticity properties of the *N*-body scattering amplitude in non-relativistic quantum mechanics," *Helv. Phys. Acta* **42** (1969), 299–329.

There is a large physics literature on various fascinating aspects of *n*-body quantum scattering beyond existence and completeness. As an introduction to this literature, the reader should consult the book of Newton quoted in the notes to Section 2, and the books by M. L. Goldberger and K. Watson, *Collision Theory*, Wiley, New York, 1964; and J. Nuttall and K. Watson, *Topics in Several Particle Dynamics*, Holden-Day, San Francisco, 1967.

Section XI.6 The technical details in the proof of Theorem XI.41 can be found in the monograph by B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1971. The proof appears primarily in Section IV.5 of the monograph although for Lemma 1, Section II.9 is needed; for Lemma 2, Section III.4 is needed; for Lemma 5, Section V.3 is needed; and Lemma 6 is found in Section V.4. The details for Theorem XI.42 can be found in Section V.5 of the monograph. For the theorem on zeros of a function analytic in the open upper half-plane, continuous in its closure, the reader should consult K. Hoffman, *Banach Spaces of Analytic Functions*, Prentice Hall, Englewood Cliffs, New Jersey, 1962.

Continuum eigenfunction expansions of the type discussed in Theorem XI.41 were first developed for ordinary differential equations in the 1940s by K. Kodaira and E. Titchmarsh, though the general idea of eigenfunction expansions goes back to the work of D. Bernoulli and J. Fourier. For a historical sketch and many references, see Dunford–Schwartz, Vol. II, p. 1581. This ordinary differential equation theory is applicable to Schrödinger operators on $\mathbb{R}^3$ with centrally symmetric potentials since such operators are direct sums of ordinary differential operators (see the appendix to Section X.1). This point of view and the resulting eigenfunction expansions have been developed by T. Green and O. Lanford III, "Rigorous derivation of the phase shift formula for the Hilbert space scattering operator of a single particle," *J. Mathematical Phys.* **1** (1960), 131–140; and J. Weidmann, "Zur Spektral theorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 268–302. See Appendix 3 to Section 8.

The earliest treatment of continuum eigenfunction expansions associated with partial differential operators is due to A. Ya. Povzner: "On the expansion of arbitrary functions in terms of the eigenfunctions of the operator $-\Delta u + cu$," *Mat. Sb.* **32** (1953), 109–156 (*Amer. Math. Soc. Trans.*, 2nd Series, **60** (1967)). The connection with scattering theory was first emphasized in A. Ya. Povzner, "On Eigenfunction expansions in terms of scattering solutions," *Dokl. Akad. Nauk SSSR* **104** (1955), and T. Ikebe, "Eigenfunction expansions associated with the Schrödinger operators and their application to scattering theory," *Arch. Rational Mech. Anal.* **5** (1960), 1–34. (Erratum: "Remarks on the orthogonality of eigenfunctions for the Schrödinger operator on $\mathbb{R}^n$," *J. Fac. Sci.*, Tokyo Univ., Sect. I, **17** (1970), 355–361.) Povzner required his potentials to have compact support.

The main idea of our proof of Theorem XI.41, namely, that the connection between the Green's function and the eigenfunctions leads via Stone's formula to (82e′), is taken from Ikebe. Ikebe's treatment differs from ours primarily in two related ways. First, he has different conditions on V: He requires only $V(r) = O(r^{-2-\epsilon})$ rather than $V \in L^1$, but his potentials must be Hölder continuous away from a finite set. Secondly, he introduces an auxiliary Banach space to contain the (unmodified) Lippmann–Schwinger function, $\varphi(x, k)$. To solve the Lippmann–Schwinger equation, he has to rely on compact operator theory in arbitrary Banach spaces, and equicontinuity arguments replace the Hilbert–Schmidt criterion in studying the kernel. The trick of factoring the potential $V = |V|^{1/2}V^{1/2}$ and using a modified Lippmann–Schwinger equation is due (independently) to H. Rollnik, "Streumaxima und gebundene Zustande," *Z. Phys.* **145** (1956), 639–653; A. Grossman and T. T. Wu (see the notes to Section 7) and J. Schwartz, "Some non-self-adjoint operators," *Comm. Pure Appl. Math.* **13** (1960), 609–639. By factoring $V = |V|^a V^{1-a}$ with $\frac{1}{4} < a < \frac{3}{4}$, one obtains a modified Lippmann–Schwinger equation with kernel that is Hilbert–Schmidt if $\int |V(x)|^{2a}|V(y)|^{2-2a}|x-y|^{-2}\,dx\,dy < \infty$ and an inhomogeneous term which is L^2 if $\int |V(x)|^{2a}\,dx < \infty$. By Sobolev's inequality, these integrals are finite if $V \in L^{3/2}$. In this way the methods of this section can be used to treat potentials that are $O(r^{-2-\epsilon})$ at ∞ (Problem 57).

Ikebe's method has been used to study Schrödinger operators in $n \neq 3$ dimensions by D. Thoe in "Eigenfunction expansions associated with Schrödinger operators in $\mathbb{R}_n$, $n \geq 4$," *Arch. Rational Mech. Anal.* **26** (1967), 335–356; and for nonlocal potentials by M. Bertero, G. Talenti, and G. A. Viano in "Eigenfunction expansions associated with Schrödinger two-particle operators," *Nuovo Cimento A* **62** (1969), 27–87. A development similar to Ikebe and Thoe but under different conditions may be found in P. Alsholm and G. Schmidt, "Spectral and scattering theory for Schrödinger operators," *Arch. Rational Mech. Anal.* **40** (1971), 281–311.

The Povzner–Ikebe eigenfunction expansion which we discuss in this section should be distinguished from the eigenfunction expansion of Gårding and Gel'fand discussed in K. Maurin, *General Eigenfunction Expansions and Unitary Representations of Topological Groups*, Polish Scientific, Warsaw, 1968. The latter type of expansion is of an abstract type associated with any operator. Its mere existence contains no spectral information; and, in fact, it consists of little more than a convenient form of the spectral theorem. On the other hand, the Povzner–Ikebe expansions contain connections with scattering theory, asymptotic completeness, and the absence of singular continuous spectrum.

Generalizations of the Povzner–Ikebe expansion to a more abstract setting, including some other elliptic differential operators, have been discussed by S. Kuroda in a series of papers: "Stationary theory of scattering and eigenfunction expansions I, II," *Sûgaku* **18** (1966), 74–85, 135–144; "Perturbation of eigenfunction expansions," *Proc. Nat. Acad. Sci. U.S.A.* **57** (1967), 1213–1217; and (the main article in the series) "An abstract stationary approach to perturbation of continuous spectra and scattering theory," *J. Analyse Math.* **20** (1967), 57–117. Kuroda's ideas and methods are closely connected with the "stationary methods" of Friedrichs which we discuss presently and with the methods of Agmon, Kuroda, and Lavine which we treat in Section XIII.8. Notice once again the element of arbitrariness in a division between "scattering theory" and "spectral properties." This work is a precursor to the abstract Kato–Kuroda theory which we discuss at the end of the notes to this section.

Our discussion of the history of eigenfunction expansions would not be complete without some reference to the general context of "stationary methods." In many ways, the "old-fashioned" naïve scattering theory which we describe later in the notes to this section is a stationary picture, but the "modern" stationary version in the physics literature is generally dated back to two important papers: B. A. Lippmann and J. Schwinger, "Variational principles for scattering processes, I," *Phys. Rev.* **79** (1950), 469–480; and M. Gell'Mann and M. L. Goldberger, "The formal theory of scattering," *Phys. Rev.* **91** (1953), 398–408. The Lippmann–Schwinger equation appeared in the first of these. The Gell'Mann–Goldberger paper suggested the use of "abelian limits," that is, the $\lim_{\epsilon \downarrow 0} \int_0^\infty e^{-\epsilon t} f'(t)\, dt$ in place of $\lim_{t \to \infty} f(t)$ (the discrete version of this limit goes back to Abel) and also contained the formula $S = 1 - 2\pi i\, \delta(E - E')T(k, k')$. These stationary methods, that is, methods which do not directly refer to a limit in *time*, have so dominated the physics literature during the past 25 years that the more natural time-dependent view of scattering is often lost! An example where the abelian limit for the wave operators exists and is unitary, even though the ordinary wave operators do not exist, can be found in J. Howland, "Banach space techniques in the perturbation theory of self-adjoint operators with continuous spectrum," *J. Math. Anal. Appl.* **20** (1967), 22–47.

T. Ikebe, in "On the phase shift formula for the scattering operator," *Pacific J. Math.* **15** (1965), 511–523, proved Theorem XI.42 for the class of potentials obeying his form of the eigenfunction expansion.

There is a second set of ideas going under the name "stationary methods" in the mathematical literature. The method and extensive references are discussed in Section X.5 of Kato's book (referred to in the notes to Section 3). Many of the ideas in the method go back to Friedrichs' 1948 paper (see the notes to Section 3). The basic equation in the theory is an integral equation which is used in the proof of the Kato–Birman theorem appearing in Kato's book. For simplicity, suppose H_0 and V are bounded, $H = H_0 + V$, and that H_0 has purely absolutely continuous spectrum. Then, if $\Omega^-(H, H_0)$ exists

$$\Omega^- = 1 + i \int_0^\infty e^{itH_0} V \Omega^- e^{-itH_0}\, dt$$

If one introduces the symbol, Γ^+ for the operation $T \mapsto \Gamma^+(T) = i \int_0^\infty e^{itH_0}Te^{-itH_0}\,dt$ when the integral exists (converging in the strong topology), then one finds the **Friedrichs' equation**

$$\Omega^- = 1 + \Gamma^+(V\Omega^-) \tag{338}$$

The point is that $\Gamma^+(T)$ has two abstract properties: (a) $T = \Gamma^+(T)H_0 - H_0\Gamma^+(T)$; (b) $\Gamma^+(T)e^{itH_0} \to 0$ strongly as $t \to \infty$. Thus $\Gamma^+(\cdot)$ can be thought of as an "inverse" of $[H_0, \cdot]$ obeying the "boundary condition" (b). The abstract properties (a) and (b) completely characterize $\Gamma^+(T)$. Using this characterization of Γ^+, it is sometimes possible to solve (338) by iteration, at least if V is "small" in some sense. Once again, there is a connection with spectral analysis. We discuss a closely connected technique in Section XIII.7.

Theorem XI.43a appeared in C. Zemach and A. Klein, "The Born expansion in nonrelativistic quantum theory, I," *Nuovo Cimento* **10** (1958), 1078–1087. The extension to n dimensions is discussed in W. Faris, "Perturbations of non-normalizable eigenvectors," *Helv. Phys. Acta* **44** (1971), 930–936, and "Time decay and the Born series," *Rocky Mountain J. Math.* **1** (1971), 637–648. Theorem XI.43b is due to M. Scadron, S. Weinberg, and J. Wright, "Functional analysis and scattering theory," *Phys. Rev.* **135** (1964), B202–B207. Related results on small coupling constant scattering theory are discussed in Sections XIII.7, XII.8, and their notes. The use of summability methods, and in particular of Padé approximants, to "sum" the Born series in regions where it diverges is discussed in J. R. Chisholm, "Solution of linear integral equations using Padé approximants and the Jost function," *Nuovo Cimento A* **61** (1969), 747–754, and J. L. Basdevant and B. W. Lee, "Padé approximation and bound states: Exponential potential," *Nuclear Phys. B* **13** (1969), 182–188.

Now, we would like to discuss the "naïve scattering theory" which goes back to M. Born, "Quantenmechanik der Stossvorgänge," *Z. Phys.* **38** (1926), 803–827. This is intended to put Theorem XI.41 in perspective and to provide a link with what the reader may have seen in quantum mechanics textbooks. In a typical scattering experiment, a beam of *nearly* constant energy E is sent into a target. Suppose that the target contains N particles. In the usual approximation, one supposes that the result is N times the scattering from a single target particle. This approximation depends on several factors which are valid in most experiments (when they are not valid, a more complicated analysis is needed): (1) The target particles are much farther apart than the "range" of the forces, that is, the characteristic falloff of the forces. The typical separation of particles in a solid target is $R_0 \cong 10^{-8}$ cm, and typical forces in nuclear experiments have a range $\cong 10^{-13}$ cm. (2) It must be a good approximation that a beam particle does not scatter off more than one target particle in going through the target. If we picture the target as being made of "sheets" 10^{-8} cm apart, the probability of scattering in any sheet is about $\sigma/\pi R^2$ where σ is the total cross section and R is the separation in the target. Since $\sigma < 10^{-25}$ cm^2 for typical nuclear experiments, this probability $\cong 10^{-9}$. Thus in a target with a thickness of 10^{-2} cm, the "probability" of a multiple collision is about 10^{-3}, so this second approximation is "typically" valid. (3) According to the picture of quantum mechanics, we cannot think of a given beam particle as scattering off a particular target particle. Rather, there are amplitudes for scattering off each target particle, and the observed amplitude is the square of the N individual amplitudes. For this to be about N times the square of a typical amplitude, we need to know that there is no interference effect. This requires the deBroglie wavelength of the beam particles λ_D to be much smaller than the interparticle separation. Again, in a nuclear experiment, if incident protons have an energy of 10 MeV, $\lambda_0 \cong 10^{-13}$, which is much smaller than R. Thus, in a typical situation, we can suppose the beam is scattering off a single target particle if we remember the right multiplicative factors involving the number densities of the target and the incident beam.

The next approximation is to suppose that the beam is "infinite" in extent. While mathematically this is somewhat severe since it leads to nonnormalized states, physically it is much milder than the approximations (1)–(3) above! Thus we picture a plane wave e^{ikz} as "input." This wave has momentum $\langle 0, 0, k\rangle$ in $\mathbb{R}^3$ (in units with $\hbar = 1$), so it represents a plane wave "entering" from $z = -\infty$. After the scattering, if we look very far from the target, we expect an outgoing wave, moving out in a spherical pattern but with an angular dependent density. If V is spherically symmetric, then for large r it should have the form $f(\theta)e^{ikr}/r$ where $f(\theta)$ is a quantity which describes the scattering. The $+$ in e^{+ikr}, which we shall see is connected with the sign in the Lippmann–Schwinger equation, is necessary for the wave to be *outgoing*, that is, for the momentum to point outward. The input beam density per unit area/per unit time is $1/v$ where v is the velocity in the particle. If we look at an area of size $r^2\, d\Omega$ about an angle θ, we observe $\{[\,|f(\theta)|^2/r^2]r^2\, d\Omega\}/v$ particles per unit time. Thus the differential cross section is given by

$$d\sigma/d\Omega = |f(\theta)|^2$$

The basic ansatz of naïve scattering theory is that the "scattering state" is an eigenfunction of the Schrödinger equation which has the asymptotic form $e^{ikz} + f(\theta)e^{ikr}/r$ *for large* r. On the surface, this ansatz looks absurd, for, if $\varphi \sim_{r\to\infty} e^{ikz} + f(\theta)r^{-1}e^{ikr}$, then *at all times* φ has both a plane wave coming in and an outgoing spherical wave. Of course we cannot expect to do better with a stationary picture! Moreover, if we consider a state which at time 0 is $\int g(k)\varphi(x, k)\, dk$, then for large r *and* t it will have the form $\int g(k)e^{ik(z-kt)}\, dk + f(\theta)r^{-1} \int g(k)e^{ik(r-kt)}\, dk$. Then, essentially by the Riemann–Lebesgue lemma, the first integral for z and t large and g peaked near k_0 has appreciable size only if $z \cong k_0 t$ and the second integral if $r \cong k_0 t$. We thus see that if $t \to -\infty$, the second integral is negligible for all r (since $r \geq 0$). Thus, we can expect to recover a time-dependent picture by forming "packets" of the naïve-type wave functions. In fact, this picture can be directly justified. See the third appendix to Section 8.

We remark that some attempts at justifying $d\sigma/d\Omega = |f(\theta)|^2$ starting from the rigorous definition of the S-operator are to be found in J. Dollard, "Scattering into cones, I: Potential scattering," *Comm. Math. Phys.* **12** (1969), 193–203; and J. Jauch, R. Lavine, and R. G. Newton, "Scattering into cones," *Helv. Phys. Acta* **45** (1972), 325–330.

The naive scattering theory method can be summarized as seeking functions $\varphi(x, k)$ that "obey" $H\varphi = k^2\varphi$ and $\varphi(x, k) \sim_{|x|\to\infty} e^{ikz} + f(\theta)r^{-1}e^{ikr}$. $f(\theta)$ is then interpreted as a function whose square gives the differential cross section. Let us present a formal derivation to show that $\varphi(x, k)$ should obey the Lippmann–Schwinger equation. Write $\varphi = e^{ikz} + \eta$. Then $(H - k^2)\varphi = 0$ implies that $(H_0 - k^2)\varphi = -V\varphi$ or $(H_0 - k^2)\eta = -V\varphi$. Thus formally $\eta = -(H_0 - k^2)^{-1}V\varphi$ or φ obeys $\varphi = e^{ikz} - (H_0 - k^2)^{-1}V\varphi$. Of course, the inverse $(H_0 - k^2)^{-1}$ is not well defined. As we shall presently see, the choice $\varphi = e^{ikz} - [H_0 - (k^2 + i0)]^{-1}V\varphi$ is directly connected with the desire that for large r, $\varphi - e^{ikz} \sim e^{ikr}r^{-1}f(\theta)$ and not $e^{-ikr}r^{-1}f(\theta)$.

We thus identify the naïve wave function φ with the Lippmann–Schwinger function. Therefore, φ obeys (with $\mathbf{k} = \langle 0, 0, k\rangle$)

$$\varphi(\mathbf{x}, k) = e^{ikz} - (4\pi)^{-1} \int e^{ik|\mathbf{x}-\mathbf{y}|}|\mathbf{x} - \mathbf{y}|^{-1}V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, dy$$

For $|\mathbf{x}|$ large, $|\mathbf{x} - \mathbf{y}|^{-1} \cong |\mathbf{x}|^{-1}$ and $\exp(ik|\mathbf{x} - \mathbf{y}|) \cong \exp(ik|\mathbf{x}| - ik \cdot \hat{\mathbf{x}}|y|) = \exp(ik|\mathbf{x}| - ik|\mathbf{y}|\cos\theta)$ where θ is the angle between x and y. Thus, formally,

$$\varphi(\mathbf{x}, \mathbf{k}) \underset{|\mathbf{x}|\to\infty}{\sim} e^{i\mathbf{k}\cdot\mathbf{x}} + |\mathbf{x}|^{-1}e^{ik|\mathbf{x}|}f(\theta)$$

where

$$f(\theta) = -(4\pi)^{-1} \int e^{-i\mathbf{k}' \cdot \mathbf{y}} V(\mathbf{y})\varphi(\mathbf{y}, \mathbf{k})\, dy = -2\pi^2 T(\mathbf{k}', \mathbf{k})$$

if $\mathbf{k}'$ is defined by $k' = k$ and $\mathbf{k} \cdot \mathbf{k}' = \cos \theta$. The above argument represents a formal justification of (96) and (97a).

Note that if we took φ to obey $\varphi = e^{ikz} - [H_0 - (k^2 - i0)]^{-1} V\varphi$, the above analysis would have led to $\varphi \sim_{r\to\infty} e^{ikz} + \tilde{f}(\theta)r^{-1}e^{-ikr}$. Our desire to have $\varphi - e^{ikz} \sim e^{+ikr}r^{-1}$ for large $|x|$ is thus directly connected with the "$+i0$ prescription" in the Lippmann–Schwinger equation.

The abstract approach to eigenfunction expansions is intimately related to the results of Section XIII.8 where the reader can find extensive references including a history. Here we note that a systematic theory has been developed by T. Kato and S. Kuroda, "Theory of simple scattering and eigenfunction expansions," in *Functional Analysis and Related Fields*, pp. 99–131, Springer-Verlag, New York, Heidelberg, Berlin, 1970. Applications of these ideas to multiparticle scattering can be found in the Howland reference in the notes to Section 5.

It is well known that the resolvent can be analytically continued in a suitable sense when the potential falls off exponentially. See, for example, the second Grossman-Wu paper quoted in the notes to Section 7, Simon's monograph quoted above, C. Dolph, J. McLeod, and D. Thoe, "The analytic continuation to the unphysical sheet of the resolvent kernal and the scattering operator associated to the Schrödinger operator," *J. Math. Anal. Appl.* **16** (1966), 311–332, or the series of papers by N. Shenk and D. Thoe, "Eigenfunction expansions and scattering theory for perturbations of $-\Delta$," *J. Math. Anal. Appl.* **36** (1971), 313-351; *Rocky Mountain J. Math.* **1** (1971), 89–125.

Section XI.7 The original motivation for study of the analytic properties of the scattering amplitude came from outside the realm of potential scattering theory. The earliest dispersion relations were proven for the index of refraction in an optical medium by R. Kronig, "On the theory of dispersion of x-rays," *J. Amer. Optical Soc.* **12** (1926), 547–558, and by H. A. Kramers, Atti del Congress Int. de Fisica, Como (1927).

In the early 1950s "dispersion theory" developed as a method of analyzing and interpreting scattering data in elementary particle physics. The progression of the development of any aspect of the theory was typically in four stages: First, a suggestion of some analyticity property was made. Next, someone found a "proof" of the property which was far from rigorous but which emphasized the physical reasons why the property should be true. Third, a rigorous proof was found in a quantum field theory framework—such rigorous proofs did not start from the Wightman axioms but from the stronger L.S.Z. framework. (Only much later was the L.S.Z. framework derived from the Wightman axioms together with additional assumptions; see Section 16 and its notes.) Finally, using some ideas from the field theory proof, a proof of the analogous property in potential scattering was developed. In some cases, stage three was never completed although stage four was successful.

The early history of dispersion theory is quite complicated and is summarized in Chapter 10 of the book of Goldberger and Watson quoted in the notes to Section 5. We note the three fundamental papers: R. Kronig, "A supplementary condition in Heisenberg's theory of elementary particles," *Physica* **12** (1946), 543-544; M. Gell'Mann, M. L. Goldberger, and W. Thirring, "Use of causality conditions in quantum theory," *Phys. Rev.* **95** (1954), 1612-1627; and M. L. Goldberger, "Use of causality conditions in quantum theory," *Phys. Rev.* **97** (1955), 508-510. This last paper contained a heuristic "derivation" of forward dispersion relations for pion-nucleon scattering. The first rigorous proof in a field theory (L.S.Z.) framework is due to K. Symanzik, "Derivation of dispersion relations for forward scattering," *Phys. Rev.* **105** (1957), 743–749. The earliest proof of a potential scattering forward dispersion relation (a weak version of Theorem XI.46) is due to N. Khuri, "Analyticity of the Schrödinger scattering amplitude and non-relativistic dispersion relations," *Phys. Rev.* **107** (1957), 1148–1156. Khuri used a Fredholm theory formulation of potential scattering due to R. Jost and A. Pais, "On the scattering of a particle by a static potential, *Phys. Rev.* **82** (1951), 840–851. Theorem XI.46 with a proof closely related to the one we give is due to A. Grossman and T. T. Wu, "Schrödinger scattering amplitude, I," *J. Mathematical Phys.* **3** (1961), 710–713.

Nonforward dispersion relations, that is, the analyticity of $f(\cdot, \Delta)$ for fixed real Δ, were first suggested by five groups of physicists approximately simultaneously: by Goldberger, Nambu and Oehme (unpublished), by Gell'Mann and Polkinghorne (unpublished), by Symanzik (unpublished), by A. Salam, "On generalized dispersion relations," *Nuovo Cimento* **3** (1956), 424–429, and by R. Capps and G. Takeda, "Dispersion relations for finite momentum-transfer pion-nuclear scattering," *Phys. Rev.* **103** (1956), 1877–1896. Rigorous field theory proofs are due to N. N. Bogoliubov, B. V. Madvedev, and M. K. Polivanov, "Probleme der Theorie der Dispersionsbeziehungen," *Fortschr. Physik* **6** (1958), 169–246; and H. Bremmerman, R. Oehme, and J. G. Taylor, "Proof of dispersion relations in quantized field theories," *Phys. Rev.* **109** (1958), 2178–2190. Discussion of analyticity in Δ for fixed k is due to H. Lehmann, "Scattering matrix and field operators," *Nuovo Cimento Suppl.* **14** (1959), 153–176. In potential scattering, the earliest version of Theorem XI.47 is due to W. Hunziker, "Regularitätseigenschaften der Streuamplitude im Fall der Potentialstreuung," *Helv. Phys. Acta* **34** (1961), 593–620. A proof using the factorization of the potential appears in A. Grossman and T. T. Wu, "Schrödinger scattering amplitude, III," *J. Mathematical Phys.* **3** (1962), 684–689.

A proof of Theorem XI.47 may be found in Chapter 6 of Simon's monograph quoted in the notes to Section 6. The only theorem explicitly stated there involves analyticity in D_α, but the proof works for any D_β with $0 < \beta \le \alpha$.

Generalized Yukawa potentials, often under the name Yukawian potentials, have been extensively studied because they are believed to be the closest nonrelativistic analogues of the situation in relativistic scattering. A summary of the various analyticity results for such potentials including a proof of Theorem XI.48 can be found in the book by V. De Alfaro and T. Regge, *Potential Scattering*, North Holland, Amsterdam, 1965. The most interesting results for Yukawian potentials involve joint analyticity in Δ and E and the related Mandelstam representation—see Section V.6 and its notes for a discussion of this theory.

In addition to the analyticity results discussed in this section there are three other broad classes of analyticity results. First, there are some analyticity results for N-body scattering—references for this may be found in the notes to Section 5. Secondly, there are results on the analyticity of individual partial wave amplitudes—these are discussed in Section 8. Finally, there are the results on analyticity in angular momentum which we briefly discuss in the notes to Section 8.

As we explained in Section 1, the physical intuition behind analyticity depends on causality. This connection is well disguised in the proofs of this section for the following reason: The causality intuition is time dependent, while our proofs used time-independent methods. The Lax–Phillips theory of Section 11 is a time-dependent framework for scattering theory based directly on causality. As a result, the analyticity properties arise naturally from the causality in the Lax–Phillips approach. However, because of technical difficulties, the Lax–Phillips theory applies to scattering in nonrelativistic quantum mechanics only for a very restricted class of potentials.

Section XI.8 References to articles which describe the theory of eigenfunction expansions for central potentials can be found in the Notes to Section 6. The development of much of the spectral analysis of Chapter XIII for this special class of potentials appears in J. Weidmann, "Zur Spektraltheorie von Sturm–Liouville Operatoren," *Math. Z.* **98** (1967), 268–302.

It is no coincidence that the scattering amplitude as found in Theorem XI.53 automatically obeys unitarity. There is a general principle that implies that when H and H_0 both have simple spectra (and this is true on each subspace of fixed angular momentum) $\Omega^{\pm}(H, H_0)$ exist, $\sigma_{ac}(H) \subset \sigma_{ac}(H_0)$, and the absolutely continuous spectrum for H_0 obeys a technical condition, then $\Omega^{\pm}(H, H_0)$ are complete. This result is discussed in Problems 87 and 88. The basic idea appears in Kuroda's *Nuovo Cimento* paper quoted in the Notes to Section 4. An error in his paper is corrected in the paper of Deift and Simon quoted in the Notes to the same section.

Theorems of the genre of Theorem XI.49 are behind Kuroda's theory of eigenfunction expansions (see the Notes to Section XI.6 and XIII.8); see especially T. Kato and S. Kuroda, "The abstract theory of scattering," *Rocky Mountain J. Math.* **1** (1971), 127–171. Our development follows closely that of T. Kato in "Scattering theory," pp. 90–113 in *Studies in Applied Math.* (A. H. Taub, ed.), Math. Assoc. Amer., Buffalo, New York, 1971. S. Kuroda, in "Scattering theory for differential operators, I," *J. Math. Soc. Japan* **25** (1973), 75–104, has shown that the fibers $T(E)$ are in certain $\mathcal{I}_p$ classes depending on the precise falloff of V. He allows slower falloff than we discuss in Theorem XI.49.

The basic connection between time delay and the phase of the quantum scattering amplitude is a discovery of L. Eisenbud, Ph.D. Thesis, Princeton Univ. 1948 (unpublished); see E. P. Wigner, "Laws/limit for the energy derivative of the scattering phase shift," *Phys. Rev.* **98** (1955), 145–147. Further discussion can be found in J. M. Jauch and J. P. Marchand, "The time delay operator for simple scattering systems," *Helv. Phys. Acta* **40** (1967), 217–229; and J. M. Jauch, K. B. Sinha, and B. N. Misra, "Time-delay in scattering processes," *Helv. Phys. Acta* **45** (1972), 398–426.

Compactness of $S(E) - I$ in certain three-body systems has been proven by R. Newton, "The three particle S-matrix," *J. Mathematical Phys.* **15** (1974), 338–343.

Like so much else, the partial wave expansion and the connection to eigenfunctions (Theorem XI.53) go back to the classic *Theory of Sound*, 2nd ed. of Lord J. W. S. Rayleigh, Macmillan, London, 1894. The use of partial wave expansions in quantum scattering was first suggested by M. Faxen and J. Holtsmark, "Beitrag zur Theorie des Durchganges langsamer Elektronen durch Gase," *Z. Phys.* **45** (1927), 307–324.

That the natural domain of convergence of Legendre series is an ellipse is a discovery of K. Neumann, *Über die Entwickelung einer Funktion mit imaginärem Argument, nach der Kugelfunktionen erster und zweiter Art*, Halla, Verlag Von Schmidt 1862; and L. W. Thome, "Über die Reihen welche Nach Kugelfunktion fortschreiten," *J. Math.* **66** (1866), 337–343. Earlier, E. Heine, "Theorie der Anziehung eines Ellipsoids," *J. Math.* **42** (1851), 70–82, had proven the basic (137). There is a long discussion of Legendre series based on the analogy with Taylor series in T. Kinoshita, J. J. Loeffel, and A. Martin, "Upper bounds for the scattering amplitude at high energy," *Phys. Rev. B* **135** (1964), 1464–1482.

The connection between ordinary differential equations and integral equations via the method of variation of parameters is a standard feature of the theory of ordinary differential equations. The closest analogue for partial differential equations is the method of Green's functions. An important difference between the situation for ordinary differential equations and that for partial differential equations is that the integral equation in the former case is a **Volterra equation** $f(x) = g(x) + \lambda \int k(x, y) f(y)\, dy$ where $k = 0$ if $x \le y$. Such equations have the property that their Neumann series $I + \lambda K + \lambda^2 K^2 + \cdots$ is convergent for all λ; in more modern terminology the operator is quasi-nilpotent, that is, $\sigma(K) = \{0\}$. It is for this reason that the possibility of an exceptional set $\mathscr{E}$ occurs in the study of the Lippmann–Schwinger equation, which corresponds to the partial differential equation—$\Delta\varphi + V\varphi = E\varphi$, but not in the study of the regular and Jost equations, which correspond to the ordinary differential equation $-u'' + Vu = Eu$.

The variable phase equation approach including extensive developments is due to F. Calegero; see especially his book, *The Variable Phase Approach to Potential Scattering*, Academic Press, New York, 1967. There is a connection between Theorems XI.55, XI.59, and the assertion of Theorem XIII.8 that $n_\ell(V)$ is the number of zeros of $u_\ell(r;\, E)$—any two imply the third. Notice that our proofs of these results use quite different methods. In particular, one can prove Levinson's theorem without recourse to analytic properties of the Jost function or the construction of Jost solutions.

A thorough discussion of partial wave amplitudes, Jost functions, etc. including the $\ell > 0$ case can be found in the monograph of V. de Alfaro and T. Regge quoted in the Notes to Section 7.

The Jost function formalism for s-wave scattering was presented in R. Jost, "Über die falschen Nullstellen der Eigenwerte der S-Matrix," *Helv. Phys. Acta* **20** (1947), 250–266; and further developed in V. Bargmann, "On the connection between phase shifts and the scattering potential," *Rev. Modern Phys.* **21** (1949), 488–493. Jost's original definition was that $\eta(k) \equiv \eta(0, k)$. The definition as a Wronskian is a later refinement especially useful for $\ell > 0$ where $x = 0$ is a singular point. The symbols $\eta(x, k)$, $\eta(k)$ are not standard; $f(x, k)$ and $f(k)$ are more usual—but since f is also used for the scattering amplitude, we have decided to use η. As we describe in the Notes to Section XIII.17, the Jost function is a (Fredholm) determinant associated with the radial Lippmann–Schwinger equation.

The behavior of $\eta(k)$ for the potential λV as a function of the coupling constant λ, especially as $\lambda \to \infty$, has been studied by K. Chadan, "The asymptotic behavior of the number of bound states of a given potential in the limit of large coupling," *Nuovo Cimento* **58** (1968), 191–204; and W. M. Frank, "Strong coupling limit in potential theory I, II," *J. Mathematical Phys.* **8** (1967), 466–476; **9** (1968), 1890–1898. Of particular interest is the connection between this behavior and the number of spherically symmetric bound states $n(\lambda V)$ of $-\Delta + \lambda V$. It is proven for a wide class of potentials that $\lim_{\lambda\to\infty} n(\lambda V)/\lambda^{1/2} = \pi^{-1} \int |V_-(x)|^{1/2}\, dx$ where $V_- = \max\{-V, 0\}$. We shall prove this by very different means in Section XIII.15.

Levinson's theorem was proven in N. Levinson, "On the uniqueness of the potential in a Schrödinger equation for a given asymptotic phase," *Danske Vid. Selsk. Mat.-Fys. Medd.* **25** (1949). For partial waves with $\ell > 0$, a detailed discussion of Levinson's theorem especially when $f(0) = 0$ (and Jost function theory in general) may be found in R. G. Newton, "Analytic properties of radial wave functions," *J. Mathematical Phys.* **1** (1960), 319–347.

The proof of Theorem XI.61 by a method similar to the one we use appears in A. Bottino, A. M. Longoni, and T. Regge, "Potential scattering for complex energy and angular momentum," *Nuovo Cimento* **23** (1962), 954–1004. A similar result, proven by a different method, appears in L. Brown, D. Fivel, B. W. Lee, and R. F. Sawyer, "Fredholm method in potential scattering and its application to complex angular momentum," *Ann. Physics* **25** (1963), 187–220.

For generalized Yukawa potentials, the discontinuities of $f_0(k^2)$ across the cut $(-\infty, -\mu_0^2)$ can be computed directly from the weight C in $\int_{\mu_0}^{\infty} C(\mu)e^{-\mu x}\, d\mu$; by an iterative procedure, one obtains the discontinuity in the interval $[-(n+1)^2\mu_0^2, -n^2\mu_0^2]$ at the nth stage. This method was developed in A. Martin, "On the analytic properties of partial wave scattering amplitudes obtained from Schrödinger's equation," *Nuovo Cimento* **14** (1959), 403–425, and "Analytic properties of $\ell \neq 0$ partial wave amplitudes for a given class of potentials," *Nuovo Cimento* **15** (1962), 99–109; it is further discussed in the book of DeAlfaro and Regge.

For generalized Yukawa potentials, the discontinuities across the cuts are especially important because $s_0(k^2)$ is polynomially bounded (in fact it approaches 1 as $k \to \infty$) so that dispersion relations can be written. This is a critical distinction from C_0^∞ potentials where the Jost function is entire (and $f_0(E)$ is meromorphic in $\mathbb{C}\backslash[0, \infty)$). In this case $s_0(k^2)$ does not have polynomial growth as $k \to \infty$.

Variational methods like the Kohn formula (136c) are of interest since they suggest that the error between a and $\beta(\psi) - (h\psi, \psi)$ is only the magnitude of the square of the error between ψ and φ. On this basis methods were developed for general phase shifts by various authors: L. Hulthén. "Variational problem for the continuous spectrum of a Schrödinger equation," *Kgl. Fys. Salla Lund Fortschn.* **14** (1944), 1-13, and W. Kohn, "Variational methods in nuclear collision problems," *Phys. Rev.* **74** (1948), 1763-1772. A third principle is due to J. Schwinger in unpublished lecture notes; the method is described in J. Blatt and J. Jackson, "On the interpretation of neutron-proton scattering data by the Schwinger variational method," *Phys. Rev.* **76** (1949), 18-37. That the principles could lead to rigorous bounds under suitable circumstances was realized by T. Kato in a series of papers, "Variational methods in collision problems," *Phys. Rev.* **80** (1950), 475, "Notes on Schwinger's variational method," *Progr. Theoret. Phys.* **6** (1951), 295-305, and "Upper and lower bounds on scattering phases," *Progr. Theoret. Phys.* **6** (1951), 394-407. The bound we give in Theorem XI.61.5 and its proof are given by L. Spruch and L. Rosenberg, "Upper bounds on scattering lengths for static potentials," *Phys. Rev.* **116** (1959), 1034-1040, and further discussed in their papers: "Upper bounds on scattering lengths for compound systems: n-D quartet scattering," *Phys. Rev.* **117** (1960), 1095-1102; "Bounds on scattering phase shifts: Static central potentials," *Phys. Rev.* **120** (1960), 474-482; "Bounds on scattering phase shifts for compound systems," *Phys. Rev.* **121** (1961), 1720-1726; and "Minimum principle for multi channel scattering," *Phys. Rev.* **125** (1962), 1407-1414. The effect of bound states on the bounds is discussed in L. Rosenberg, L. Spruch, and T. O'Malley, "Upper bounds on scattering lengths when composite bound states exist," *Phys. Rev.* **118** (1960), 184-192. Rosenberg-Spruch note that their bounds also can be proven with the methods Kato used earlier. The reader may have noticed that while (136d) is a lower bound, Rosenberg-Spruch refer to an upper bound. This is because they use the opposite sign convention for a from the one we use. Their convention, which makes the scattering length of a hard sphere positive (and equal to its radius), is slightly more common in the literature than ours, but both conventions are frequently used.

There is a rather large literature on oscillatory potentials. Discussion of scattering for noncentral potentials with severe oscillations at infinity (of the kind occurring in Example 1 of Appendix 2) can be found in V. B. Matveev and M. M. Skriganov, "Wave operators for the Schrödinger equation with rapidly oscillating potential," *Dokl. Akad. Nauk SSSR* **202** (1972), 755-758, M. M. Skriganov, "Spectrum of the Schrödinger operator with strongly oscillating potentials," *Trudy. Stek. Math.* **125** (1973), 183-195; M. Combescure and J. Ginibre, "Spectral and scattering theory for the Schrödinger operator with strongly oscillating potentials," *Ann. Inst. H. Poincaré Sect. A* **24** (1976), 17-29; M. Schechter, "Spectral and scattering theory for elliptic operators of arbitrary order," *Comment. Math. Helv.* **49** (1974), 84-113, and "Scattering theory for the Schrödinger equation with potentials not of short range," Jubilee Volume Dedicated to the 70th Anniversary of Academician I. N. Vekua, USSR Acad. Sci., 1977. In particular, the quadratic form construction outlined in Example 1 is due independently to Combescure, Ginibre, and Schechter. These authors also derive stronger results in the scattering theory for these potentials than appear in the text by using the methods of Section XIII.8.

Because of Pearson's example (see Section 4), there has been discussion of oscillations near zero, see, for example, W. O. Amrein and V. Georgescu, "Strong asymptotic completeness of wave operators for highly singular potentials," *Helv. Phys. Acta* **47** (1974), 517-533; and M. L. Baetman and K. Chadan, "Scattering theory with highly singular oscillating potentials," *Ann. Inst. H. Poincaré Sect. A* **24** (1976), 1-16. These local oscillations can be controlled by the method of Theorem XI.68. In particular, Baetman and Chadan analyze the regular integral equation with oscillatory potentials in much the same way we analyze the Jost equation in Example 1, revisited. In fact, we have closely followed their approach, concentrating on $r = \infty$ in place of $r = 0$. The absence of positive eigenvalues in this case (Theorem XI.68a) seems to be a new result although it could have been proven by Baetman and Chadan had they considered oscillations at infinity.

Parts (a) and (c) of Theorem XI.67 are due to F. Atkinson, "The asymptotic solutions of second order differential equations," *Ann. Mat. Pura Appl.* **37** (1954), 347–378.

Theorem XI.66 is due to J. Dollard and C. Friedman, "On strong product integration," *J. Functional Analysis* **28** (1978), 309–354. Their application to recover some of Atkinson's results and also Theorem XI.67b appears in their paper, "Product integrals and the Schrödinger equation," *J. Mathematical Phys.* **18** (1977), 1598–1607.

Theorem XI.69 is an abstraction of an argument of T. A. Green and O. E. Lanford, III, "Rigourous derivation of phase shift formula for the Hilbert space scattering operator of a single particle," *J. Mathematical Phys.* **1** (1960), 139–148. These authors also go further to allow potentials in Corollary 1 with $|V(x)| \le C|x|^{-1-\epsilon}$; they do this by considering higher order contributions in the Jost solution series. The application of the theory in combination with Theorem XI.67 is due to J. Dollard and C. Friedman, "Existence of the Møller wave operators for $r^{-\beta}\lambda \sin(\mu r^{\alpha})$," *Ann. Phys.* **111** (1978), 251–266.

Existence and completeness of the wave operators, but only for sufficiently high energies, for noncentral potentials with behavior like $r^{-1} \sin r$ at infinity has been obtained by K. Mochizuki and J. Uchiyama, 1977 Nagoya Institute of Technology, preprint.

The results of the appendices show how subtle the phenomenon of positive eigenvalues really is. For example, suppose that $V(r) \sim Cr^{-1} \sin(r^{\alpha})$ for large r. If $\alpha < 1$, then $\partial V/\partial r = O(r^{-1-\epsilon})$, so no positive eigenvalues can occur by Theorem XIII.58. If $\alpha > 1$, then $\int_x^\infty V(r)\, dr = O(r^{-1-\epsilon})$, so no positive eigenvalues can occur by Theorem XI.68. It is only for $\alpha = 1$ that such eigenvalues can occur and then they actually do occur sometimes.

We close the notes of this section, our last on short-range nonrelativistic quantum scattering with a brief description of *some* of the topics which we have *not* touched upon in the text or notes:

(1) One of the most interesting is the theory of analytic continuation of the quantities $f_\ell(E)$ in ℓ. This idea is due to T. Regge, "Introduction to complex orbital momenta," *Nuovo Cimento* **14** (1959), 951–976; and is further discussed by R. G. Newton, *The Complex J-Plane: Complex Angular Momentum in Non-Relativistic Quantum Scattering Theory*, Benjamin, New York, 1964. For an introduction to the use of the method in particle physics, see P. D. B. Collins and E. U. Squires, *Regge Poles in Particle Physics*, Springer-Verlag, New York, Heidelberg, Berlin, 1968.

(2) The "inverse problem" of reconstructing the potential given $\delta_\ell(k)$; the basic paper is that of I. M. Gel'fand and R. M. Levitan, "On the determination of a differential equation from its spectral function," *Izv. Akad. Nauk SSSR Ser. Math.* **15** (1951), 309–360; for a more complete history and a discussion of the Gel'fand–Levitan method, see Chapter 12 of the Regge–deAlfaro monograph. For lucid reviews, including more recent work, see Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory*, Gordon and Breach, New York, 1963; L. D. Faddeev, "The inverse problem in the quantum theory of scattering," *J. Mathematical Phys.* **4** (1963), 72–104; L. D. Faddeev, "Properties of the *S*-matrix of the one dimensional Schrödinger equation," *Trudy. Mat. Inst. Steklov* **73** (1964), 314–333 (*Amer. Math. Soc. Transl.* **65**, 139–166) and J. J. Loeffel, "On an inverse problem in potential scattering theory," *Ann. Inst. H. Poincaré Sect. A* **8** (1968), 339–447. A beautiful new approach to the inverse problem can be found in P. Deift and E. Trubowitz, "Inverse scattering on the line," *Comm. Pure Appl. Math.* **32** (1979) (to appear).

(3) The *N/D* method of G. Chew and S. Mandelstam, "Theory of low-energy pion-pion interaction," *Phys. Rev.* **119** (1963), 467–477.

(4) General methods for obtaining information from the analyticity properties of multiparticle scattering amplitudes. This is especially relevant in relativistic scattering theory, but is also of interest in the nonrelativistic theory. For a mathematical discussion, see A. Martin, *Scattering Theory: Unitarity, Analyticity and Crossing*, Lecture Notes in Physics, Number 3, Springer-Verlag, New York, Heidelberg, Berlin, 1969. For discussions emphasizing applications to particle physics and/or the connections with quantum field perturbation theory, see G. Chew, *The Analytic S-Matrix*, Benjamin, New York, 1966; R. J. Eden, *High Energy Collisions of Elementary Particles*, Cambridge Univ. Press, London and New York, 1967; and R. J. Eden, P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, *The Analytic S-Matrix*, Cambridge Univ. Press, London and New York, 1966.

Section XI.9 Classical Coulomb scattering was first developed by Lord Rutherford as part of his famous experiment which led to the conclusion that atoms had nuclei. Rutherford was very lucky, for the quantum Coulomb cross section just happens to exactly equal the classical one (this miracle is further compounded in that the Born approximation is exact in this case!). Moreover, he was lucky in that the α particles he used were not energetic enough to significantly interact with the nucleus through nuclear forces, so he saw only the Coulomb interaction.

For a discussion of exact solutions of the classical Coulomb problem from a symmetry (Lenz vector) point of view, see H. Abarbanel, "The inverse r-squared force: An introduction to its symmetries," in *Studies in Mathematical Physics, Essays in Honor of Valentine Bargmann* (E. Lieb, B. Simon, A. Wightman, eds.), Princeton Univ. Press, Princeton, New Jersey, 1976.

Long-range classical scattering theory from the point of view we use was developed by I. Herbst, "Classical scattering with long range forces," *Comm. Math. Phys.* **35** (1974), 193–214. All of Theorem XI.73 except for the parts involving (165) are due to Herbst. The discussion of "asymptotically central" potentials is new.

Quantum Coulomb scattering was first treated by W. Gordon, "Über den Stoss zweier Punktladungen nach der Wellenmechanik," *Z. Phys.* **48** (1928), 180–191, who dealt with the eigenfunction expansion for the Coulomb problem working a priori with the time-independent formalism. He found that the continuum eigenfunctions did not look like

$$e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\theta)$$

for r large, but rather like

$$e^{i\mathbf{k}\cdot\mathbf{r}} + r^{-1}\exp(i[kr + \lambda k^{-1}\ln(4kr)])f_{\text{E}}(\theta)$$

for r large and $\theta \neq 0$, and identified $f_{\text{E}}(\theta)$ with the Coulomb scattering amplitude. He thus eliminated the infinite phase shifts by fiat.

The time-dependent theory of quantum Coulomb scattering appeared first in J. Dollard, "Asymptotic convergence and the Coulomb interaction," *J. Mathematical Phys.* **5** (1964), 729–738. We use the symbol $U_{\text{D}}(t)$ for this reason. His results were extended to more general long-range potentials by W. O. Amrein, Ph. A. Martin, and B. Misra, "On the asymptotic condition in scattering theory," *Helv. Phys. Acta* **43** (1970), 313–344; V. S. Buslaev and V. B. Matveev, "Wave operators for the Schrödinger equation with a slowly decreasing potential," *Theoret. and Math. Phys.* **2** (1970), 266–274; P. K. Alsholm and T. Kato, "Scattering with long range potentials," in *Partial Differential Equations*, pp. 393–399, Proc. Symp. Pure Math., Vol. 23, Amer. Math. Soc., Providence, Rhode Island, 1973; and by L. Hörmander, "The existence of wave operators in scattering theory," *Math. Z.* **146** (1976), 69–91. Amrein et al. extended Dollard's method to allow $r^{-\alpha}$ potentials for $\alpha > \frac{1}{2}$. Buslaev–Matveev and Alsholm–Kato use high order approximate solutions to the Hamilton–Jacobi equation and require information on higher and higher derivatives as the range gets longer and longer; for example, Buslaev-Matveev require $|D^\alpha V_l(x)| \le C(1 + x)^{-\epsilon-|\alpha|}$ for all $|\alpha| \le k$ where $k = [n/2] + 2 + [1/\varepsilon]$ where $[a] \equiv$ largest integer less than a. The strongest result is due to Hörmander whose paper includes Theorem XI.84. Hörmander dealt with general constant coefficient differential operators for H_0.

Dollard and Hörmander discuss multichannel problems.

Eigenfunction expansions for the purely Coulomb case are discussed in Dollard's paper. Eigenfunctions for general long-range potentials are part of the general subject of spectral analysis of such potentials, and some references can be found in the notes to Section XIII.8. Recent work on the subject includes: T. Ikebe, "Spectral representations for Schrödinger operators with long-range potentials," *J. Functional Analysis* **20** (1975), 158–177; and "Spectral representations for Schrödinger operators with long-range potentials—Perturbation by short-range potentials," *Publ. Res. Inst. Math. Sci.* **11** (1976), 551–558; T. Ikebe and H. Isozaki, "Completeness of modified wave operators for long range potentials," *Pub. RIMS Kyoto* **14** (1978), (to appear); H. Isozaki, "On the long range wave operators," *Publ. Res. Inst. Math. Sci. Pub. RIMS Kyoto* **13** (1977), 589–626; H. Kitada, "Scattering theory for Schrödinger operators with long-range potentials, I, II," *J. Math. Soc. Jap.* **29** (1977), 665–691; G. Pinchuk, "Abstract time independent wave operator theory for long-range potentials," Berkeley thesis, unpublished; Y. Saito, "Eigenfunction expansions for the Schrödinger operator with long-range potentials, $Q(y) = O(|y|^{-\epsilon})$, $\varepsilon > 0$," *Osaka J. Math.* **14** (1977), 37–53. In addition S. Agmon has announced fairly complete results exploiting extensions of his weighted L^2-space techniques. Finally, V. Enss has informed us that his methods described in Section 17 can be modified to accommodate long range potentials including the Coulomb potential.

The quantum on-energy-shell S-operators for long-range potentials typically are very singular at $k = k'$ (zero scattering angle). In the short-range case, the distribution $s(k, k')$ has only a $\delta(k - k')$ singularity at $k = k'$; in the Coulomb case the singularity is worse; see I. Herbst, "On the connectedness structure of the Coulomb S-matrix," *Comm. Math. Phys.* **35** (1974), 181–191.

Finally, we want to make some remarks about the phase of the Coulomb scattering amplitude. As we have carefully explained, the phase is not determined by the basic time-dependent theory. Nevertheless, there is a sense in which this phase is measurable! To understand this phenomenon we shall have to say something about how dispersion relations are experimentally checked; more information on this of relevance to our discussion can be found in R. Eden, *High Energy Collisions of Elementary Particles*, Cambridge Univ. Press, London and New York, 1967.

One would like to check forward dispersion relations in strongly interacting systems. The problem with doing this is that the only reasonable targets are charged particles, namely the protons in a hydrogen target. Moreover, the easiest projectiles to detect after scattering are charged, say π^+. Since the particles are charged, there are Coulomb forces as well as strong interactions, and an infinite cross section results due to very small angle Coulomb scattering. How does one try to find the "strong part" of the scattering amplitude to check the forward dispersion relations? Physicists make the ansatz:

$$f(\theta) = f_s(\theta) + f_c(\theta) \tag{339}$$

where $f_c(\theta)$ is the "standard" Coulomb amplitude as found by Gordon. We discuss this ansatz further below. Typically, the differential cross section at small angles looks like the solid line in

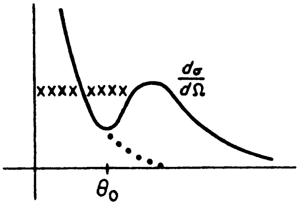


FIGURE XI.18

the schematic Figure XI.18. The dotted line represents the exact value of $|f_c|^2$. How do we "find" $\operatorname{Im} f_s(\theta = 0)$ and $\operatorname{Re} f_s(\theta = 0)$? In the region when f_c is very small, the differential cross section is essentially $|f_s(\theta)|^2$. The crossed line in Figure XI.18 represents an extrapolation of the putative $|f_s(\theta)|^2$ to $\theta = 0$. By integrating this over θ and using the optical theorem, one deduces what $\operatorname{Im} f_s(\theta = 0)$ is. How do we find $\operatorname{Re} f_s(\theta = 0)$? One expects $f_s(\theta)$ to be slowly varying near $\theta = 0$, so we need only find $\operatorname{Re} f_s(\theta = \theta_0)$. The dip at $\theta = \theta_0$ is caused by interference between f_s and f_c at the point where $|f_s| \sim |f_c|$. The magnitude of the dip *and the knowledge of* f_c allow one to find the argument of f_s, and so $\operatorname{Re} f_s(\theta = \theta_0)$. With this, one can check the forward dispersion relations. The point is that if one believes forward dispersion relations, one can turn around the analysis and "measure" the argument of f_c. How does this fit in with the fact that this argument is not determined by the usual time-dependent theory? The key seems to be (339) and the demand of forward dispersion relations. The f_s in (339) will not be the true scattering amplitude for the strong interaction since f is *not* linear in the potential. We thus regard (339) as a definition of f_s. Namely, we *conjecture* the following: With the choice of modified quantum dynamics we made in the Coulomb case (which Dollard arranged to yield the "usual" Coulomb amplitude if $V_s = 0$) for any central sufficiently short-range potential, the function $f(k, \theta; \lambda r^{-1} + V_s) - f(k, \theta; \lambda r^{-1})$ has a limit $g(k)$ as $\theta \to 0$ which is the boundary value of a function analytic and polynomially bounded in the cut plane $\mathbb{C}\backslash[0, \infty)$ with $g(\bar{k}) = \overline{g(k)}$. Moreover, this is not true for any other Dollard dynamics leading to *different* phases. A proof of this conjecture would explain why Gordon's phase is "the right one."

Section XI.10 The idea of formulating the scattering for wave equations as a Hilbert space problem goes back at least as far as M. Birman, "Existence conditions for wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **27** (1963), 883-906 (*Amer. Math. Soc. Trans., Ser. 2* **54** (1966), 91-117); and P. Lax and R. Phillips, "The wave equation in exterior domains," *Bull. Amer. Math. Soc.* **68** (1962), 47-49. The necessity of dealing with unitary groups on different spaces was first pointed out by C. Wilcox in "Wave operators and asymptotic solutions of wave propagation problems of classical physics," *Arch. Rational Mech. Anal.* **37** (1966), 37-78. We have mainly followed the general ideas in T. Kato, "Scattering theory with two Hilbert spaces," *J. Functional Analysis* **1** (1967), 342-369. In particular, Theorems XI.75 and XI.76 in case $\mathcal{H}_0 = \mathcal{H}_1$ are contained in Kato's paper including the case where B_0 or B_1 has a nontrivial null space. Kato introduced the notion of equivalence of identification operators and has repeatedly emphasized that on physical grounds certain identification operators are more natural than others.

The details for our sketch of existence and completeness of the wave operators in the case of optical scattering in an inhomogeneous medium (Example 2) can be found in M. Reed and B. Simon, "The scattering of classical waves from inhomogeneous media," *Math. Z.* **155** (1977), 163-180. The construction in the text of the wave operators for Maxwell's equations proves convergence in a norm distinct from the usual energy norm. This can be remedied by looking at the wave equations for the vector potentials. See, for example, the paper just mentioned.

Scattering from obstacles (Example 3) using the point of view of this section is discussed in C. Wilcox, *Scattering Theory for the d'Alembert Equation in Exterior Domains*, Lecture Notes in Math. **442**, Springer-Verlag, New York, Heidelberg, Berlin, 1975; and P. Deift, *Classical Scattering Theory with a Trace Condition*, Princeton Univ. Press, Princeton, New Jersey, 1979. Additional references for scattering from obstacles appear in the notes to Section 11.

The first proofs of asymptotic completeness for acoustical and optical scattering in inhomogeneous media were given independently by M. S. Birman, "Scattering problems for differential operators with perturbations of the space," *Izv. Akad. Nauk SSSR Ser. Mat.* **35** (1971), 440–455; and by J. Schulenberger and C. Wilcox, Completeness of the wave operators for perturbations of uniformly propagative systems," *J. Functional Anal.* **7** (1971), 447–472. Results in certain very special cases were already proven in M. S. Birman, "Existence conditions for wave operators," *Izv. Akad. Nauk SSSR Ser. Mat.* **27** (1963), 883–906 (*Amer. Math. Soc. Trans., Ser. 2* **54** (1966), 91–117). The 1971 Birman paper and the Schulenberger–Wilcox paper required a certain amount of smoothness on the coefficients. The smoothness conditions were removed in V. G. Deič, "Application of the method of nuclear perturbations in two-space scattering theory," *Izv. Vysš. Učebn. Zaved. Fizika* (1971); and J. Schulenberger, "A local compactness theorem for wave propagation problems of classical physics," *Indiana Univ. Math. J.* **22** (1972), 429–432. The idea that we discuss, using the commutation formula to remove smoothness conditions, is due to P. Deift.

The approach of Schulenberger–Wilcox is different from ours in that they reduce second order wave equations to systems that are first order in the space variables as well as the time variable. For example, in the case of acoustic scattering, if u satisfies (187), then

$$v(x) \equiv \left\langle \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \frac{\partial u}{\partial x_3}, \frac{\partial u}{\partial t} \right\rangle$$

satisfies

$$\frac{\partial v}{\partial t} = E(x)^{-1}\left(\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i}\right) v \equiv i\Lambda v \tag{340}$$

where

$$E(x) = \begin{pmatrix} \rho(x) & 0 & 0 & 0 \\ 0 & \rho(x) & 0 & 0 \\ 0 & 0 & \rho(x) & 0 \\ 0 & 0 & 0 & 1/\rho(x)c(x)^2 \end{pmatrix}$$

and the A_i are constant matrices so that

$$\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i} = \begin{pmatrix} 0 & 0 & 0 & \partial/\partial x_1 \\ 0 & 0 & 0 & \partial/\partial x_2 \\ 0 & 0 & 0 & \partial/\partial x_3 \\ \partial/\partial x_1 & \partial/\partial x_2 & \partial/\partial x_3 & 0 \end{pmatrix}$$

Similarly, one writes the free equation as

$$\frac{\partial v}{\partial t} = E_0^{-1}\left(\sum_{i=1}^{3} A_i \frac{\partial}{\partial x_i}\right) v \equiv i\Lambda_0 v \tag{341}$$

where E_0 is a constant matrix. In his 1966 paper, Wilcox initiated a study of the scattering theory for general first-order systems of the form (340), (341), where:

(i) E_0, $E(x)$, A_i are self-adjoint.
(ii) E_0 and $E(x)$ are strictly positive definite with

$$0 < e_0 \leq E(x) \leq e_1$$

(iii) The roots of $\det(\lambda E_0 - \sum_{i=1}^{n} A_i p_i)$ have constant multiplicity and constant sign for $p \in \mathbb{R}^n \backslash \{0\}$.
(iv) $E(x) \to E_0$ sufficiently rapidly as $|x| \to \infty$.

Wilcox called systems with a slightly stronger condition "uniformly propagative" and proved the existence of the wave operators. The acoustic equation, Maxwell's equations in isotropic media, and many other classical equations are uniformly propagative. For many results, condition (iii) can be replaced by the weaker condition that $\operatorname{rank}(\sum_1^n A_i p_i)$ be independent of p for $p \in \mathbb{R}\backslash\{0\}$. Such systems of "constant deficit" include Maxwell's equations in general inhomogeneous media. However, completeness was left open since neither the Birman–Belopol'skii theorem, nor Kato's reduction to a single Hilbert space problem was available.

The Birman–Belopol'skii theorem (Theorem XI.13) was proven in M. S. Birman and A. L. Belopol'skii, "The existence of wave operators in scattering theory for a pair of spaces," *Math. USSR-Izv.* **2** (1968), 117–1130. And, in "Some applications of a local criterion for the existence of wave operators," *Soviet Math. Dokl.* **10** (1969), 393–397, M. S. Birman pointed out that the Birman–Belopol'skii theorem can be used to prove completeness in a system of the form (340), (341), *if* $\sum A_i\, \partial/\partial x_i$ is elliptic. Unfortunately, the first-order systems corresponding to the acoustic wave equation and Maxwell's equations are not elliptic since $\sum A_i p_i$ has zero as an eigenvalue. Schulenberger and Wilcox then showed in their 1971 paper that if one had a coerciveness estimate, then the Birman–Belopol'skii theorem could be extended to the case where there are zero modes. In "Coerciveness inequalities for non-elliptic systems of partial differential equations," *Ann. Mat. Pura Appl.* **88** (1971), 229–305, Schulenberger and Wilcox proved the necessary estimates, thus concluding the proof of completeness for acoustic and optical scattering in inhomogeneous media. Their proof of the coerciveness inequalities was greatly simplified by T. Kato in "On a coerciveness theorem of Schulenberg and Wilcox," *Indiana Univ. J. Math.* **25** (1975), 979–985. See also Deift's book. Birman's 1971 approach to the problem avoided coerciveness estimates but still used local compactness. Recently, in his book, P. Deift has shown that coerciveness inequalities and local compactness can be avoided completely. He uses the more general invariance principle discussed in the notes to Section 3, which says that if

$$\frac{\Lambda_0^n}{(\Lambda_0 + ia)^{2n}} - \frac{\Lambda^n}{(\Lambda + ia)^{2n}} \in \mathscr{I}_1 \tag{342}$$

for each $a \neq 0$, then existence and completeness of the wave operators follows. He is then able to verify (342) since the zero modes are projected out by Λ_0 and Λ.

The Agmon–Kuroda method (see Section XIII.8) has been extended to treat systems like those occurring in this section in T. Kako, "Scattering theory for abstract differential equations of the second order," *J. Fac. Sci. Univ. Tokyo Sect. IA Math.* **19** (1972), 377–392.

For the acoustic wave equation, the problem of the zero modes is an entirely unnecessary difficulty which appears only if one reduces to a first-order equation in the space derivatives. By reducing to first-order only in the time derivative as we did in Example 1, one keeps ellipticity and the Kato reduction-to-one-Hilbert space method or the Birman–Belopol'skii theorem can be applied directly. In the case of Maxwell's equations one is presented with a nonelliptic system first-order in the space and time variables. But, as indicated in Example 2, this can easily be turned into a second-order (nonelliptic) system. By adding the missing part of the Laplacian one can make the system elliptic by giving the zero modes some nontrivial dynamics. The ellipticity and the Kato reduction theory then give completeness. Since this dynamics decouples from the dynamics of the nonzero modes, the scattering theory for the nonzero modes is not affected. For details, see the Reed–Simon paper. The moral is: If you've got ellipticity, keep it; if you ain't got it, get it.

Trace class results under change of boundary condition go back to M. S. Birman, "Perturbations of the continuous spectrum of a singular elliptic operator under the change of the boundary and boundary conditions," *Vestnik Leningrad. Univ. Mat. Meh. Astronom.* **1** (1962), 22–55. Theorem XI.79 is proven using Wiener integral methods in the Deift–Simon paper quoted in the notes to Section 4; see also B. Simon, *Functional Integration and Quantum Physics*, Academic Press, New York, 1979. Theorems XI.80 and XI.81 are taken from Deift's monograph quoted above; our development follows many of his ideas. His proof of Theorem XI.81, which is very different from our proof of the special case, uses results of A. Calderón, "Lebesgue spaces of differentiable functions and distributions," *Proc. Symp. Pure Appl. Math.* **4** (1961), 33–49, Amer. Math. Soc., Providence, Rhode Island. Deift discusses the more general case of acoustic operators with both obstacles and inhomogeneities. He also remarks that Theorem XI.81 does not handle a case of physical interest where Γ is a piece of hyperplane ("diffraction experiment"). One can, however, modify our proof of Theorem XI.81 to cover this case (Problem 119). Deift develops an alternative theory which works in cases where one can only prove that $\tilde{R}_{\Gamma \cup S;N}$ is compact, a result which is connected with the Rellich-type theorems of Section XIII.14. His idea is (in the notation of the appendix) to prove that $R_{\Gamma,N}^2 \chi$ and χR_0^2 are compact and that $R_{\Gamma,N}^2(1-\chi) - (1-\chi)R_0^2$ is trace class. The second result implies the existence of the wave operators, $\Omega^{\pm}(H_{\Gamma;N}, H_0, 1-\chi)$, and the first implies that $1-\chi$ is asymptotically equivalent to the identity.

The idea for Lemma 6 in the proof of Theorem XI.81′ is borrowed from F. Guerra, L. Rosen, and B. Simon, "Boundary conditions for the $P(\varphi)_2$ Euclidean field theory," *Ann. Inst. H. Poincaré Sect. A* **25** (1976), 231–334, who use a similar method in the proof of certain technical estimates relating $R_{\Gamma;N}$ to R_0.

Section XI.11 The basic reference for the approach to scattering theory described in this section is P. D. Lax and R. S. Phillips, *Scattering Theory*, Academic Press, New York, 1967. The representation theorem (Theorem XI.82) which provides the link between incoming and outgoing subspaces and the scattering operator was first stated and proved by Ja. Sinai, "Dynamical systems with countable Lebesgue spectrum, I," *Izv. Akad. Nauk SSSR Ser. Mat.* **25** (1961), 899–924. Sinai deduced the theorem from von Neumann's uniqueness theorem (Theorem XI.84). Lax and Phillips gave a proof from first principles: They first prove the discrete version (Theorem XI.83) and then obtain a spectral representation on $L^2[0, 2\pi; N]$ by the Fourier transform. Using complex analysis and the Cayley transform they obtain a spectral representation on $L^2(-\infty, \infty, N)$ for the continuous case, and then the inverse Fourier transform yields Theorem XI.82. The proof which we give is patterned after ideas in Mackey's imprimitivity theorem. The connection of this theorem to von Neumann's theorem goes back at least to G. W. Mackey, "A theorem of Stone and von Neumann," *Duke Math. J.* **16** (1949), 313–326, and is further discussed in his book *Induced Representations of Groups and Quantum Mechanics*, Benjamin, New York, 1968. References for von Neumann's theorem may be found in the notes to Section VIII.5; an alternative proof is outlined in Problem 30 of Chapter X. Our proof of the lemma to Theorem XI.82 is modeled on von Neumann's celebrated proof of the uniqueness of

Haar measure: J. von Neumann, "The uniqueness of Haar's measure," *Mat. Sb.* **1** (1936), 721–734.

There are connections between ergodic theory and Theorems XI.82 and XI.83 made by Kolmogorov and Sinai, which account for Sinai's interest in the theorems. To see the connection, consider the Baker's transformation (Example 2 of Section VII.4). If D_+ is the space of functions of x alone with $\int f\,dx = 0$, then D_+ can be seen to be an outgoing subspace for U restricted to $\{1\}^\perp$, yielding a proof that U is mixing. Theorem XI.82 is relevant for the continuous case. Indeed, one defines a **K-system** as a measure space $\langle \Omega, \Sigma, \mu \rangle$ with $\mu(\Omega) = 1$, a one-parameter group T_t of measure preserving transformations and a subalgebra Σ_+ of Σ so that (i) $T_t[\Sigma_+] \subset \Sigma_+$ for $t > 0$; (ii) the largest σ-algebra contained in all $T_t[\Sigma_+]$ is $\{\emptyset, \Omega\}$; (iii) the smallest σ-algebra containing all the $T_t[\Sigma_+]$ is Σ. If one takes $\mathscr{H} = \{f \in L^2 \mid \int f\,d\mu = 0\}$, $D_+ = \{f \in \mathscr{H} \mid f \text{ is } \Sigma_+ \text{ measurable}\}$ and $U(t)f = f \circ T_t^{-1}$, then D_+ is an outgoing subspace and, in particular T_t is mixing.

In their book, Lax and Phillips use the scattering of acoustical waves by an obstacle with Dirichlet boundary conditions (Example 3) as the main example to illustrate the application of their general theorems. Their theory also applies to Neumann and certain other boundary conditions. We have used scattering from inhomogeneous media to illustrate the general theory in order to facilitate comparison with the techniques of Section 10. Because of interest in the connection between the geometry of the obstacle, local energy decay, and the poles of the scattering operator (see below), obstacle scattering in homogeneous media has been the main problem discussed in the literature, though many authors have noted that their results extend to inhomogeneous media. The inhomogeneous case is explicitly treated using the Lax–Phillips theory in J. LaVita, J. Schulenberger, and C. Wilcox, "The scattering theory of Lax and Phillips and wave propagation problems of classical physics," *ONR Tech. Rep.* **16** (1971).

Theorem XI.89 is a special case of a general theorem of Y. Foures and I. Segal, "Causality and analyticity," *Trans. Amer. Math. Soc.* **78** (1955), 385–405. A proof of Fatou's theorem may be found in Chapter 11 of P. Duren, *Theory of H^p Spaces*, Academic Press, New York, 1970. The original idea goes back to P. Fatou, "Series trigonométriques et séries de Taylor," *Acta Math.* **30** (1906), 335–400, who treated the case of a bounded analytic function in a disk. The scattering operator $s(z)$ in the Lax–Phillips book is analytic in the *lower* half-plane because they use the plus sign for the Fourier transform while we use the minus sign. For proofs of Theorems XI.90 and XI.91 which connect the poles of $s(z)$ to the spectrum of B, see the book by Lax and Phillips. The statements of results are different since they write semigroups as $Z(t) = e^{Bt}$ while we write semigroups as e^{-Bt}. Thus their B has spectrum in the left half-plane and ours has spectrum in the right half-plane.

The poles of the scattering operator are closely connected with physical observation, so it is important to investigate their positions in the lower half-plane. According to Theorem XI.90, this problem reduces to studying $\sigma(B)$. By using a functional calculus for B, the conclusion of Theorem XI.91 can be strengthened in various ways by adding more hypotheses:

Theorem Suppose that the hypotheses of Theorem XI.91 hold. Then,

(a) If for some T, $\|Z(T)\| = a < 1$, then

$$\sigma(B) \subset \left\{ z \,\middle|\, \operatorname{Re} z \geq -\frac{\ln a}{T} \right\}$$

(b) If $Z(T)$ is compact for some T, then for every $c > 0$ there are only finitely many points of $\sigma(B)$ in the set $\{z \mid \operatorname{Re} z < c\}$.

(c) If for some T the range of $Z(T)$ lies in $D(B)$, then there exist $a \in \mathbb{R}$, $b > 0$ so that

$$\sigma(B) \subset \left\{ z \,\middle|\, \operatorname{Re} z > a + b \ln|z| \right\}$$

Conditions (a) and (b) were given by Lax and Phillips in their book. They also showed that condition (b) implies the existence of an asymptotic series in the energy norm of a solution in a bounded region; the series is a sum of exponentials with rates depending on positions of the poles. Because of this, condition (b) is particularly important to verify in applications. Condition (c) was stated and verified in P. Lax and R. S. Phillips, "A logarithmic bound on the location of the poles of the scattering matrix," *Arch. Rational Mech. Anal.* **40** (1971), 268–280, for the equation $u_{tt} - c(x)^2 \Delta u - q(x)u = 0$ under a variety of hypotheses. C. S. Morawetz and D. Ludwig, "The generalized Huygens' principle for reflecting bodies," *Comm. Pure Appl. Math.* **22** (1969), 189–205, prove a general Huygens' principle for the propagation of singularities and energy decay for scattering from a convex body (Dirichlet boundary conditions) and use the result to verify (b). Another proof of (b) using their Huygens' principle appears in R. S. Phillips, "A remark on the preceding paper of C. S. Morawetz and D. Ludwig," *Comm. Pure Appl. Math.* **22** (1969), 207–211. In C. S. Morawetz, "The decay of solutions of the exterior initial-boundary value problem for the wave equation," *Comm. Pure Appl. Math.* **14** (1961), 561–568, and "The limiting amplitude principle," *Comm. Pure Appl. Math.* **15** (1962), 349–361, it was shown that the energy decays uniformly like t^{-1} in bounded regions exterior to a star-shaped obstacle; and P. Lax, C. S. Morawetz, and R. S. Phillips, "Exponential decay of solutions of the wave equation in the exterior of a star-shaped obstacle," *Comm. Pure Appl. Math.* **16** (1963), 477–486, then showed that this implies an exponential rate of decay. This in turn implies that $\|Z(t)\varphi\| \leq ce^{-\alpha t}\|\varphi\|$, so (a) holds in the case of a star-shaped obstacle.

Notice that our verification of the hypotheses of Theorem XI.91 in Example 3 used the fact that the local energy decays, but uniformity was not required nor were any special geometric conditions required of the obstacle. On the other hand, to get uniform decay one would expect some geometric condition (as the above titles suggest) since if the obstacle is too badly dented, it should be possible to trap energy in its vicinity for arbitrarily long times by appropriate choices of initial conditions. In their book, Lax and Phillips conjecture that if the sojourn times of light rays in the neighborhood of the obstacle are unbounded above, then $\|Z(t)\| = 1$ for all t. The conjecture was verified by J. Ralston in "Solutions of the wave equation with localized energy," *Comm. Pure Appl. Math.* **22** (1969), 807–823. In "Trapped rays in spherically symmetric media and poles of the scattering matrix," *Comm. Pure Appl. Math.* **24** (1971), 571–582, Ralston shows that the same is true in the inhomogeneous case if $c(x)$ wiggles too much at ∞. Lax and Phillips also conjectured that if the sojourn times are bounded, then $Z(t)$ is eventually compact, which in particular would imply that $\|Z(t)\|$ is eventually less than one by (223). This weaker form of the conjecture has been proven in C. Morawetz, J. Ralston, and W. Strauss, "Decay for solutions of wave equations outside of non-trapping obstacles," *Comm. Pure Appl. Math.* **30** (1977), 447–508. This connection between the geometry of the obstacle and the poles of the scattering operator via energy decay estimates is one of the most beautiful aspects of the Lax–Phillips method. In this connection, C. S. Morawetz and D. Ludwig, "An inequality for the reduced wave operator and the justification of geometrical optics," *Comm. Pure Appl. Math.* **21** (1968), 187–203, show that the formal solution of the scattering problem given by geometrical optics is asymptotic to the exact solution given by the Lax–Phillips theory. For other results on the position of the poles of $s(z)$, see P. Lax and R. S. Phillips, "Decaying modes for the wave equation in the exterior of an obstacle," *Comm. Pure Appl. Math.* **22** (1969), 737–787; and "On the scattering frequencies for the Laplace operator for exterior domains," *Comm. Pure Appl. Math.* **25** (1972), 85–101.

The application of their method to quantum scattering is described by Lax and Phillips in their book and further developed in P. D. Lax and R. S. Phillips, "The acoustic equation with an indefinite energy form," *J. Functional Analysis* **1** (1967), 37–83. See also C. Dolph, J. McLeod, and D. Thoe, "The analytic continuation to the unphysical sheet of the resolvent kernel and the scattering operator associated with the Schrödinger equation," *J. Math. Anal. Appl.* **16** (1966), 311–332.

In their book Lax and Phillips also present two proofs (one due to M. Schiffer) that the obstacle (Dirichlet conditions) is uniquely determined by the scattering operator. This has been extended by A. Majda who shows in "High frequency asymptotics for the scattering matrix and the inverse problem of acoustical scattering," *Comm. Pure Appl. Math.* **29** (1976), 261–291, and "A representation formula for the scattering operator and the inverse problem for arbitrary bodies" *Comm. Pure Appl., Math.* **30** (1977), 165–194, that a convex hull obstacle is already determined through an explicit formula by the high frequency asymptotics of the kernel $k(\theta, w; \sigma)$ of $I - \hat{S}$. Majda's results have been extended by P. Lax and R. S. Phillips, "Scattering of sound waves from an obstacle," *Comm. Pure Appl. Math.* **30** (1977), 195–233.

The Lax–Phillips approach has been extended and applied to a variety of other situations than those we have discussed: For even dimensions, see P. Lax and R. S. Phillips, "Scattering theory for the acoustic equation in an even number of space dimensions," *Indiana Univ. Math. J.* **22** (1972), 101–134. For symmetric hyperbolic systems with conserved energy, see P. D. Lax and R. S. Phillips, "Scattering theory," *Rocky Mountain J. Math.* **1** (1971), 173–223. For dissipative hyperbolic systems, see P. D. Lax and R. S. Phillips, "Scattering theory for dissipative hyperbolic systems," *J. Functional Analysis* **14** (1973), 172–236; and C. Foias, "On the Lax–Phillips nonconservative scattering theory," *J. Functional Analysis* **19** (1975), 272–301. For moving obstacles, see J. Cooper and W. Strauss, "Energy boundedness and decay of waves reflected off a moving boundary," *Indiana Univ. Math. J.* **25** (1976), 671–690. For an application to transport phenomena, see P. D. Lax and R. S. Phillips, "Scattering theory for transport phenomena," in *Functional Analysis* (B. Gelbaum, ed.), Thompson, 1967. Scattering in certain non-Euclidean geometries which leads to S-matrices that are connected to automorphic functions are studied in L. Faddeev and B. S. Pavlov, "Scattering theory and automorphic functions," *Sem. Steklov Inst. Math. Leningrad* **27** (1972), 161–193, and P. Lax and R. S. Phillips, *Scattering Theory for Automorphic Functions*, Ann. Math. Stud. **87**, Princeton Univ. Press, Princeton, New Jersey, 1976.

The twisting trick of the appendix is due to E. B. Davies and B. Simon in their paper quoted in the notes to Section 4. They discuss the Neumann boundary condition case and several other applications.

Section XI.12 The material in this section is based on three papers: J. Hejtmanek, "Scattering theory of the linear Boltzmann operator," *Comm. Math. Phys.* **43** (1974), 109–120; B. Simon, "Existence of the scattering matrix for the linearized Boltzmann equation," *Comm. Math. Phys.* **41** (1975), 99–108; and J. Voigt, "On the existence of the scattering operator for the linear Boltzmann equation," *J. Math. Anal. Appl.* **58** (1977), 541–558. See also V. Protopopescu, "On the scattering matrix for the linear Boltzmann equation," *Rev. Roumaine Phys.* **21** (1976), 991–994.

Hejtmanek (whose paper was the first to appear in preprint form) isolated the problem and proved the basic solvability result in Theorem XI.93 including assertions (a)–(c) and Theorem XI.94. Simon introduced the lemma appearing before Theorem XI.94, proved Theorem XI.95 under the stronger hypothesis (diam $D)(M(\sigma_a) + M(\sigma_p)) < 1$, and proved Theorem XII.96 under this same hypothesis. Simon remarks that these ideas are closely related to the theory of smooth perturbations discussed in Section XIII.7. Simon's paper also contains an example showing that the dynamics may not be invertible on L^1_+. Voigt proved the estimate in Theorem XI.93d and Theorems XI.95 and XI.96 under the hypotheses we use. He also extended these results to some cases of noncompact support and gave an example of a regular subcritical pair for which $\tilde{\Omega}^-$ fails to exist.

The general (that is, nonlinear) Boltzmann equation was suggested by L. Boltzmann, "Uber die Aufstellung und Integration der Gleichungen, welche die Molekularbewegung in Casen bestimmen," *Sitz. Wien.* **74** (1876), 503. For recent discussion of mathematical problems associated with this equation, see E. G. D. Cohen and W. Thirring. *The Boltzmann Equation*, Springer; Vienna, 1973. The linearized Boltzmann equation has been used extensively to study phenomena very different from those we discuss: for those transport phenomena associated with reactors, see I. Bell and S. Glasston, *Nuclear Reactor Theory*, Van Nostrand, Princeton, New Jersey, 1970; for transport phenomena in stars, D. Mihalas, *Stellar Atmospheres*, Freeman, San Francisco, 1970.

Section XI.13 The first results on the scattering theory of the equation

$$u_{tt} - \Delta u + m^2 u = -gu^3 \tag{343}$$

were proven in I. Segal, "Quantization and dispersion for nonlinear relativistic wave equations," *Proc. Conf. Mathematical Theory of Elementary Particles (Dedham, Mass. 1965)*, pp. 79–108, MIT Press, Cambridge, Massachusetts. Segal showed that for all sufficiently nice solutions u_- of the free equation, there is a solution u of (343) such that $u_- - u \to 0$ as $t \to -\infty$. Similarly for each u_+, a u exists. Thus, Segal constructed the wave operators $\Omega^\pm$ on certain sets of nice data. In "Dispersion for nonlinear relativistic wave equations," *Ann. Sci. École Norm. Sup.* **1** (1968), 459–497, Segal showed that if u_- and u_+ are small (or g is small), then $\Omega^\pm$ can be inverted so the scattering operator exists for small data. This paper contains most of the small data scattering ideas we have presented. Small data methods were then applied by J. Chadam to more general equations in "Asymptotics for $\Box u = m^2 u + G(x, t, u, u_x, u_t)$, I, II," *Ann. Scuola Norm. Sup. Pisa Fis. Mat.* **26** (1972), 33–65, 67–95; and by W. von Wahl for the case $m = 0$ in "Uber die klassische Lösbarkeit des Cauchyproblems für nichtlineare Wellengleichungen bei kleinen Anfangswerten und das asymptotische Verhalten der Lösungen," *Math. Z.* **114** (1970), 281–299. The abstract low energy scattering theory that we present follows closely the outline in W. Strauss, "Nonlinear scattering theory," in *Scattering Theory in Mathematical Physics* (J. Lavita and J.-P. Marchand, eds.), Reidel, Dordrecht, The Netherlands, 1974. The proof that we give of Theorem XI.98 includes several additional improvements of Strauss.

Our proof of Theorem XI.101 is closely patterned after the original proof of W. Strauss, "Decay and asymptotics for $\Box u = F(u)$," *J. Functional Analysis* **2** (1968), 409–457. The idea of proving a decay estimate by integrating by parts and identifying positive terms in a conserved quantity goes back at least to C. Morawetz, "The limiting amplitude principle," *Comm. Pure Appl. Math.* **15** (1963), 349–361. Asymptotic completeness for (343) for the case $m > 0$ is much harder to prove than in the case $m = 0$. Although there is a broken conformal charge, similar to that in Problem 153, the source term is positive, which ruins the decay estimate. For the $m > 0$ case, where $g = g(x)$ is small at ∞, Strauss constructed Ω^+ and Ω^- in "Decay of solutions of hyperbolic equations with localized nonlinear terms," *Symposia Mathematica*, Vol. VII, *Probleme di Evoluzione*, Instituto Nazionale di Alta Matematica (Roma), Academic Press, New York, 1971, 339–355. Then C. Morawetz and W. Strauss proved asymptotic completeness for $m > 0$, g a positive constant, in "Decay and scattering of solutions of a nonlinear relativistic wave equation," *Comm. Pure Appl. Math.* **25** (1972), 1–31. Their proof, which is quite difficult, successively improves a weak decay estimate which had previously been obtained by C. Morawetz in "Time decay for the Klein–Gordon equation," *Proc. Roy. Soc. London Ser. A* **30G** (1968), 291–296. An abstract version of their proof appears in M. Reed, "Construction of the scattering operator for abstract nonlinear wave equations," *Indiana Univ. Math. J.* **25** (1976), 1017–1027. Further properties of the scattering operator are proven in C. Morawetz and W. Strauss, "On a nonlinear scattering operator," *Comm. Pure Appl. Math.* **26** (1973), 47–54.

Asymptotic completeness for the nonlinear Schrödinger equation

$$i\, du/dt = (-\Delta + m)u + f(u)$$

for various nonlinear terms $f(u)$ has been proven in J. E. Lin and W. Strauss, "Decay and scattering of solutions of the nonlinear Schrödinger equation," *J. Functional Analysis* **30** (1978), and in a series of papers by J. Ginibre and G. Velo, "On a class of non-linear Schrödinger equations," I and II, *J. Functional Analysis*, to appear; III, *Ann. Institut Poincaré* **28** (1978), 287–316. To obtain the necessary a priori decay estimate, Ginibre and Velo use a broken invariance analogously to the use of the broken conformal invariance described in Problem 153.

There is an extensive literature on this subject. For references and further discussion, see M. Reed, *Abstract Non-linear Wave Equations*, Lecture Notes in Mathematics **507**, Springer-Verlag, New York, Heidelberg, Berlin, 1976, and Strauss's "Non-linear scattering theory" lectures referred to above, and his "Invariant wave equations" lectures referred to below.

A discussion of bound states in nonlinear systems and, in particular, the details of the example can be found in W. Strauss, "Existence of solitary waves in higher dimensions," *Commun. Math. Phys.* **55** (1977), 149–162, where references are given to earlier work.

There has been extensive study of a special class of equations, including the Korteweg–de Vries equation and the sine-Gordon equation, which have bound states with very special properties. Namely, there is no scattering between channels. That is, a state that looks like n solitons at $t = -\infty$ will also look like n solitons at $t = +\infty$. Indeed, the velocities of the solitons will even be the same. For an introduction to the literature, see C. Scott, F. Chu, D. McLaughlin, "The soliton: A new concept in applied science," *Proc. IEEE* **61** (1973), 1443–1483; and *Nonlinear Wave Motion* (A. Newell, ed.), Lectures in Applied Mathematics **15**, Amer. Math. Soc., Providence, Rhode Island, 1974

Noether's theorem goes back to E. Noether, "Invariante Variationsprobleme," *Nachr. Akad. Wiss. Göttingen Math-Phys.* (kl. II) (1918), 235–257. These ideas have become a standard part of classical field theory; see, for example the treatment in N. Bogoliubov and D. Shirkov, *Introduction to the Theory of Quantized Fields*, Wiley (Interscience), New York, 1959. That invariants of the dynamics are connected with groups of transformations commuting with the dynamics is an idea that is familiar from classical and quantum mechanics. Let $T_t^{(H)}$ be the flow on phase space generated by a Hamiltonian $H(p, q)$ through the Hamilton equations (X.153). If $T_t^{(f)}$ is the flow generated by $f(p, q)$ and $T_t^{(H)}T_s^{(f)} = T_t^{(f)}T_s^{(H)}$, then f is invariant under $T_t^{(H)}$, that is, $f(T_t^{(H)}\langle p, q\rangle) = f(p, q)$. In quantum mechanics, let H be the Hamiltonian and A another self-adjoint operator. If e^{-isH} and e^{-itA} commute, then the spectral measures of A are invariant under e^{-itH}, that is,

$$(E_\Omega^{(A)} e^{-itH}\varphi, e^{-itH}\varphi) = (E_\Omega^{(A)}\varphi, \varphi) \qquad \text{for all } \varphi \text{ and } t$$

Notice, however, two things about the classical field theory case. First, it is more convenient to work in the Lagrangian formulation than in the Hamiltonian formulation. Secondly, the conserved quantities appear as the integrals of local densities.

For a different but related approach to finding conserved quantities and many references, see W. Strauss's lectures, "Nonlinear invariant wave equations," in *Invariant Wave Equations*, Springer Lecture Notes in Physics **73** (1978), 197–249.

The group of fractional linear transformations on $\mathbb{C}$ is generated, geometrically, by rotations, translations, dilations, and inversion on $\mathbb{R}^2$. Analogously, the group of transformations of $\mathbb{R}^4$

generated by rotations, translations, dilations, and the inversion $x \to x/x \cdot x$ is called the conformal group because it too preserves angles. If we continue t to it, the rotation group becomes the Lorentz group and the inversion becomes the Lorentz inversion; this is the group that physicists usually refer to as the conformal group. It preserves angles in the Lorentz inner product.

Section XI.14 The notion of magnons was first developed in the physics literature in connection with theories of ferromagnetism. We do not intend to give any complete discussion of the rather extensive literature on the subject or on the Heisenberg model in general, but we mention the instructive article of F. Dyson, "General theory of spin-wave interactions," *Phys. Rev.* **102** (1956), 1217–1230; and a collection of reprints on *Ferromagnetism* published by the Physical Society of Japan.

The basic ideas for scattering in the zero-temperature Heisenberg model are due to G. J. Watts, "Theory of spin-wave scattering," Ph.D. Thesis, Bedford College, 1973; and K. Hepp, "Scattering theory in the Heisenberg ferromagnet," *Phys. Rev. B* **5** (1972), 95–97. A comprehensive review can be found in R. F. Streater, "Spin-wave scattering" in *Scattering Theory in Mathematical Physics* (J. A. LaVita and J. P. Marchand, eds.), pp. 273–298, Reidel, Dordrecht, The Netherlands, 1974.

Bound states of magnons are discussed in J. G. Hanus, "Bound states in the Heisenberg ferromagnet," *Phys. Rev. Lett.* **11** (1963), 336–337; and M. Wortis, "Bound states of two spin waves in the Heisenberg ferromagnet," *Phys. Rev.* **132** (1963), 85–97.

One can study magnon scattering in the one-dimensional Heisenberg model at a much more detailed level since it is possible to obtain many formulas in closed form. In particular, for each n, there is exactly one n-magnon bound state. The reason this model is so tractable is that, like solitons in one dimension, the spin waves do not scatter off one another, nor is there transfer of momentum. For more details, see L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, I," *J. Math. Anal. Appl.* **59** (1977), 392–414; D. Babbitt and L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, II. An explicit Plancherel formula," *Comm. Math. Phys.* **54** (1977), 255–278; and D. Babbitt and L. Thomas, "Ground state representation of the infinite one-dimensional Heisenberg ferromagnet, III. Scattering theory," *J. Mathematical Phys.*, **19** (1978), 1699–1704.

The Hilbert space that we constructed in the infinite volume case can also be realized as an infinite tensor product. Let

$$D_0 = \left\{ \bigotimes_{\alpha \in \mathbf{Z}^3} v_\alpha \,\middle|\, v_\alpha \in \mathbf{C}^2,\ \text{all but finitely many } v_\alpha \text{ equal } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

where we define a linear structure so that $\otimes v_\alpha$ is linear in each v_α when all the others are fixed. For v and w in D_0 with $v = \otimes v_\alpha$, $w = \otimes w_\alpha$, we define

$$(v, w) = \prod_{\alpha \in \mathbf{Z}^3} (v_\alpha, w_\alpha)_{\mathbf{C}^2} \tag{344}$$

The product makes sense since all but finitely many terms are equal to one. Moreover, (344) extended to be sesquilinear can be shown to define an inner product on D_0 (Problem 136). Then, the completion of D_0 in the inner product is a Hilbert space which is one of an uncountable set of distinct tensor products we can construct by replacing $\binom{0}{1}$ by different sequences. This space is isomorphic to $\mathscr{H}$ under the map $\psi(\{\alpha_\beta\}) \mapsto \otimes v_\beta$ where $v_\beta = \binom{0}{1}$ (respectively, $\binom{1}{0}$) if $\alpha_\beta = 0$ (respectively, 1). Infinite tensor products were introduced by J. von Neumann in "On infinite direct products," *Compositio Math.* **6** (1938), 1–77. For a summary, see the appendix in M. Reed, "Self-adjointness in infinite tensor product spaces," *J. Functional Analysis* **5** (1970), 94–124.

Section XI.15 The mathematical treatment of quantum field scattering in an external field has its roots in the work of R. Feynman, "The theory of positrons," *Phys. Rev.* **76** (1949), 749–759; A. Salam and P. Matthews, "Fredholm theory of scattering in a given time-dependent field," *Phys. Rev.* **90** (1953), 690–695; and J. Schwinger, "Theory of quantized fields, IV, V," *Phys. Rev.* **92** (1953), 1283–1299; **93** (1954), 615–628. All four papers deal with electron–positron scattering in a given external classical electromagnetic field. Feynman wrote down successive approximations to certain scattering amplitudes in terms of classical propagators and discussed the connection between his formulas, the hole theory of Dirac, and second quantization. The papers of Salam–Matthews and Schwinger write down what was implicit in Feynman's paper, namely, Dyson-type expansions for the scattering operator in terms of the in field and the external field, and study the convergence of the expressions for certain matrix elements.

The realization of Yukawa field theories as an integral over external fields was developed on a formal level by A. Salam and P. Matthews, "The Green's functions of quantized fields," *Nuovo Cimento* **12** (1954), 563–565; "Propagators of quantized fields," *Nuovo Cimento* **2** (1955), 120–134. For the two-dimensional theory, the formalism was put on a rigorous footing by E. Seiler, "Schwinger functions for the Yukawa model in two dimensions with space–time cutoff," *Comm. Math. Phys.* **42** (1975), 153–182. See also, E. Seiler and B. Simon, "Nelson's symmetry and all that in the $(\text{Yukawa})_2$ and $(\varphi^4)_3$ field theories," *Ann. Physics* **97** (1976), 476–518. This formalism has been responsible for much recent progress including verification of the Wightman axioms for small coupling.

The first attempt to develop the entire mathematical apparatus for external field problems in a fully rigorous way was made by A. Capri, "Electron scattering in a given time-dependent electromagnetic field," *J. Mathematical Phys.* **10** (1969), 575–580. Capri pointed out that the construction of the dynamics for the field could be completely reduced to constructing the analogous classical dynamics. However, Capri's proof of the existence of the out-vacuum was inconclusive. This difficulty was remedied in B. Schroer, R. Seiler, and J. Swieca, "Problems of stability for quantum fields in external time-dependent potentials," *Phys. Rev. D* **2** (1970), 2927–2937, where spins other than $\frac{1}{2}$ are also discussed. The development of the theory in the spin zero (coupling of (278)) and spin $\frac{1}{2}$ cases was summarized in R. Seiler, "Quantum theory of particles with spin zero and one half in external fields," *Comm. Math. Phys.* **25** (1972), 127–151. We have followed in part the presentation in Seiler's paper.

Additional references on the external field problem include: J. Bellissard, "Quantized fields in interaction with external fields; I. Exact solutions and perturbation expansion; II. Existence theorems," *Comm. Math. Phys.* **41** (1975), 235–266; **46** (1976), 53–74; P. Bongaarts and S. Ruijsenaars, "The Klein paradox as a many particle problem," *Ann. Physics* **101** (1976), 289–318; J. M. Chadam, "Unitarity of dynamical propagators of perturbed Klein–Gordon equations," *J. Mathematical Phys.* **9** (1968), 386–396; W. Hochstenbach, "Field theory with an external potential," *Comm. Math. Phys.* **51** (1976), 211–217; M. Klaus and G. Scharf, "The regular external field problem in quantum electrodynamics," *Helv. Phys. Acta* **50** (1977), 779–802 and "Vacuum polarization in Fock space," *Helv. Phys. Acta* **50** (1977), 803–814; L. E. Lundberg, "Relativistic quantum theory for charged spinless particles in external vector fields," *Comm. Math. Phys.* **31** (1973), 295–316; J. Palmer, "Scattering automorphisms of the Dirac field," *J. Functional Analysis*, to appear, and "Symplectic groups and the Klein–Gordon field," *J. Math. Anal. and Appl.*, to appear; S. Ruijsenaars, "Charged particles in external fields; I. Classical theory; II. The quantized Dirac and Klein Gordon theories," *J. Mathematical Phys.* **18** (1977), 720–737, *Comm. Math. Phys.* **52** 1977), 267–294, and the collection of articles in *Invariant Wave Equations* (G. Velo and A. S. Wightman, eds.), Springer Lecture Notes in Physics **73**, Berlin, Heidelberg, New York, 1978.

Theorem XI.108 is due to D. Shale, "Linear symmetries of free boson fields," *Trans. Amer. Math. Soc.* **103** (1962), 149–167. The analogous theorem for fermions was proven in D. Shale and W. Stinespring, "Spinor representations of infinite orthogonal groups," *J. Math. Mech.* **14** (1965), 315–322. Both papers depend on results in I. Segal, "Distributions in Hilbert space and canonical systems of operators," *Trans. Amer. Math. Soc.* **88** (1958), 12–41. There is a large literature on Bogoliubov transformations; see, for example, R. Powers and E. Størmer, "Free states of the canonical anti-commutation relations," *Comm. Math. Phys.* **16** (1970), 1–33; K. Fredenhagen, "Implementation of automorphisms and derivations of the CAR algebra," *Comm. Math. Phys.* **52** (1977), 255–266; and G. Labonté, "On the nature of strong Bogoliubov transformations for fermions," *Comm. Math. Phys.* **36** (1974), 59–72 for the fermion case, P. Kristensen, L. Mejlbo, and E. T. Poulsen, "Tempered distributions in infinitely many dimensions, III: Linear transformations of field operators," *Comm. Math. Phys.* **6** (1967), 29–48; A. Klein, "Quadratic expressions in a free Boson field," *Trans. Amer. Math. Soc.* **181** (1973), 439–456; and F. Berezin, *The Method of Second Quantization*, Academic Press, New York, 1966, for the Boson case; and S. Ruijsenaars, "On Bogoliubov transformations, I, II," *J. Mathematical Phys.* **18** (1977), 517–526, and *Ann. Phys.* (to appear).

There is an equivalent formalism for Bogoliubov transformations called the symplectic transformation approach. This is the approach used by Segal and Shale, in particular. It is more compact, mathematically more elegant, and it makes contact with various problems in group representations and number theory; however, explicit calculations of the kind we make in the text are often easier in the Bogoliubov formalism.

To describe the symplectic transformation approach, we recall that the Segal field operator $\Phi_S(f)$ of Section X.7 was defined over any complex Hilbert space $\mathscr{H}$ but that $f \to \Phi_S(f)$ was only *real* linear. The canonical commutation relations took the form

$$[\Phi_S(f), \Phi_S(g)] = i\,\mathrm{Im}(f, g)_{\mathscr{H}}$$

A symplectic transformation is a *real* linear map $T\colon \mathscr{H} \to \mathscr{H}$ so that

$$\mathrm{Im}(Tf, Tg) = \mathrm{Im}(f, g) \tag{345a}$$

If one lets T^t be the adjoint of T as a map on the real Hilbert space $\mathscr{H}_r$ with inner product $(f, g)_r = \mathrm{Re}(f, g)$, then (345a) is equivalent to

$$T^t J T = J \tag{345b}$$

where J is multiplication by i. If one picks a complex conjugation C, then one can write $\mathscr{H}_r = \mathscr{K} \oplus J\mathscr{K}$ where $\mathscr{K}$ is the real subspace $\mathscr{K} = \{\varphi \mid C\varphi = \varphi\}$. In terms of this direct sum $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ and (345b) can be recognized as the usual symplectic transformation condition if $\dim \mathscr{H} < \infty$. The symplectic transformations induce a natural transformed field

$$(\mathscr{T}\Phi)_S(f) = \Phi_S(Tf) \tag{346}$$

Since

$$a^\dagger(f) = \frac{1}{\sqrt{2}}[\Phi_S(f) - i\Phi_S(Jf)]$$

$$a(Cf) = \frac{1}{\sqrt{2}}[\Phi_S(f) + i\Phi_S(Jf)]$$

we see that (346) is equivalent to (301) if we take

$$
\begin{aligned}
(\mathscr{T}\Phi)_S(f) &= \frac{1}{\sqrt{2}}\,[a_B^\dagger(f) + a_B(Cf)] \\
B_+ = \frac{1}{2}[T - JTJ], &\qquad B_- = \frac{C}{2}[T + JTJ]
\end{aligned}
\tag{347}
$$

Notice that $B_\pm$ are complex linear and that (298) is equivalent to (345). The inverse formulas (299), (300) are equivalent to $T^{-1} = -JT^tJ$ which holds if T is invertible (a priori it may have only a left inverse).

Shale's original implementability theorem says that if T is an invertible symplectic transformation, then there exists a unitary U_T so that

$$U_T\Phi_S U_T^{-1} = (\mathscr{T}\Phi)_S$$

if and only if $T^tT - 1$ is Hilbert–Schmidt. But, by (347) and (345b),

$$T^tT - 1 = 2TCB_- \tag{348}$$

so that Shale's criterion is equivalent to the $B_- \in \mathscr{I}_2$ criterion we state since $2T^tC$ is invertible. Shale's proof is somewhat different from that we give and proceeds by first writing a real polar decomposition $T = Q|T|$, with $|T| = \sqrt{T^tT}$. The orthogonal symplectic transformation Q is explicitly implementable by the operator $\Gamma(Q)$ equal to $Q \otimes \cdots \otimes Q$ on $\Gamma_n(\mathscr{H})$; in Bogoliubov transform language, $B(Q)_- = 0$ by (348) so $B(Q)_+$ is unitary and $\Gamma(U)a^\dagger(f)\Gamma(U)^{-1} = a^\dagger(Uf)$ trivially. Thus, one need only prove the theorem in the case $T > 0$. In that case, one can formally realize T as a scale transformation S_T on Q space and write an explicit formula for a unitary inducing T by $(Uf)(q) = N_T(q)f(S_Tq)$ where $N_T(q)^2$ is a Jacobian for the change of variables. The condition $T^tT - 1 \in \mathscr{I}_2$ is needed to show that $N_T(q)$ is well defined.

Shale's theorem in case $T^t = T$ is equivalent to asking when two Gaussian processes are mutually absolutely continuous; this is discussed in Section I.6 of B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton Univ. Press, Princeton, New Jersey, 1974. These results are well known in the probability literature and predate the work of Shale; see J. Feldman, "Equivalence and perpendicularity of Gaussian Processes," *Pacific J. Math.* **8** (1958), 699–708, and J. Hajek, "On a property of the normal distribution of any stochastic process," *Czech. Math. Z.*, **8** (1958), 610–618 (Selected translation in *Math. Stat. Prob.* **1** (1961) 245–256).

For the coupling that we used in the section, we could have carried through the theory with a single Hermitian scalar field. For other couplings it is often necessary to use the charged field.

The smoothness hypothesis on $V(x, t)$ which we made in the section were convenient but not crucial. However, some kind of smallness condition on V as $|x| \to \infty$ and $|t| \to \infty$ is necessary for our simple approach to go through. First, suppose that $V(x, t) = \alpha(t)$ and that $\alpha(\cdot)$ has compact support in t, that is, we turn on and then turn off a constant scalar field. Then we can define the interacting dynamics as in the section obtaining at each time t a representation of the canonical commutation relations $a(x, t)$, $b^\dagger(x, t)$; but we cannot expect this dynamics to be unitarily implemented since turning on $\alpha(t)$ is the same as changing the mass. And, even for free fields, changing the mass means changing the representation of the canonical commutation relations (Theorem X.46). The physical reason for this is that since the potential is infinitely extended, it can create infinitely many pairs in a finite time. On the other hand, suppose that $V(x, t) = \beta(x)$ is independent of time. Then even if $\beta(x)$ is localized in space, it is not clear how to define the out-fields or the out-dynamics. And, certainly one would not expect in general the out representation of the canonical commutation relations to be unitarily equivalent to the in fields since the potential has time to create infinitely many pairs. Using the machinery of Banach algebras, P. Bongaarts in "The electron–positron field, coupled to external electromagnetic potentials, as an elementary C^* algebra theory," *Ann. Physics* **56** (1970), 108–139, has shown how to define the outfields in the case of the Dirac equation in a static external field. For certain very special cases he obtains unitary implementability. These difficulties in the *linear* external field problems, where there are no problems of multiplying operator-valued distributions together, show how hard the dynamics for fully nonlinear field theories really are.

There has been a considerable amount of work on the external field problem for higher spin equations ($s > 1$) where, in all known cases, there are additional difficulties. First, it is sometimes difficult to choose an appropriate positive definite inner product on the space of solutions—the positive definiteness is needed for second quantization. If one changes the inner product to force it to be positive definite, then one loses the commutation relations for the corresponding propagated field. Secondly, G. Velo and D. Zwanziger in "Propagation and quantization of Rarita–Schwinger waves in an external electromagnetic potential," *Phys. Rev.* **186** (1969), 1337–1341, and "Noncausality and other defects of interaction Lagrangians for particles of spin one and higher," *Phys. Rev.* **188** (1969), 2218–2222, discovered that certain formally Lorentz invariant equations have a noncausal propagation. What they showed was this: Call a fundamental solution "causal" if it has support in the forward light cone and "weakly causal" if it decays faster than any power in spacelike directions. Velo and Zwanziger showed for certain equations that *if* they have a weakly causal fundamental solution, then it is *not* causal. Recently L. Gårding has shown that there are equations and external fields for which no weakly causal fundamental solutions exist. There are still further diseases. Several lucid review articles have been written by A. S. Wightman: Introductory remarks in *Troubles in the External Field Problem for Invariant Wave Equations* (A. S. Wightman, reviewer), Gordon and Breach, New York, 1971; "Relativistic wave equations as singular hyperbolic systems," *Proc. Symp. Pure Math.* **XXIII**, pp. 441–447, Amer. Math. Soc., 1973; "Instability phenomena in the external field problem for two classes of relativistic wave equations," in *Essays in Honor of Valentine Bargmann*, pp. 423–460, Princeton Univ. Press, Princeton, New Jersey, 1976.

There is a large literature on potential scattering for the Dirac and Klein–Gordon equations. For the Dirac equation, the reader can consult K. J. Eckhardt, "On the existence of wave operators for Dirac operators," *Manuscripta Math.* **11** (1974), 349–371; and "Scattering theory for Dirac operators," *Math. Z.* **139** (1974), 105–131; J. C. Guillot and G. Schmidt, "Spectral and scattering theory for Dirac operators," *Arch. Rational Mech. Anal.* 55 (1974), 193–206; K. Mochinzuki, "On the perturbation of the continuous spectrum of the Dirac operator," *Proc. Japan Acad.* **40** (1964), 707–712; R. Prosser, "Relativistic potential scattering," *J. Mathematical Phys.* **4** (1963), 1048–1054; M. Thompson, "Eigenfunction expansions and the associated scattering theory for potential perturbations of the Dirac equation," *Quart. J. Math. Oxford Ser.* **23** (1972), 17–55; the Veselic–Weidmann papers quoted in the Notes to Section 4; R. A. Weder, "Spectral properties of the Dirac Hamiltonian," *Ann. Soc. Sci. Bruxelles Sér. I* **87** (1973), 341–355; and O. Yamada, "On the principle of limiting absorption for the Dirac operator," *Publ. Res. Inst. Math. Sci.* **8** (1972/73), 557–577. For the Klein–Gordon theory, the references include, J. M. Chadam, "The asymptotic behavior of the Klein–Gordon equation with external potential, I, II," *J. Math. Anal. Appl.* **31** (1970), 334–348; *Pacific J. Math.* **31** (1969), 19–31; Deift's monograph quoted in the notes to Section 10; T. Kako, "Spectral and scattering theory for the j-self-adjoint operators associated with the perturbed Klein–Gordon type equations," *J. Fac. Sci. Univ. Tokyo Sect IA Math.* **23** (1976), 199–221; L. Lundberg, "Spectral and scattering theory for the Klein–Gordon equation," *Comm. Math. Phys.* **31** (1973), 243–257; M. Schechter, "The Klein–Gordon equation and scattering theory," *Ann. Physics* **101** (1976), 601–609 (see also Schechter's papers on elliptic systems quoted in the Notes to Section XIII.8 and the second of his papers quoted in the Notes to Section 3); W. Strauss, "Scattering for hyperbolic equations," *Trans. Amer. Math. Soc.* **108** (1963), 13–37; D. Thoe, "Spectral theory for the wave equation with a potential term," *Arch. Rational Mech. Anal.* **22** (1966), 364–406; K. Veselic, "A spectral theory for the Klein–Gordon equation with an external electrostatic potential," *Nuclear Phys. A* **147** (1970), 215–224; R. Weder, "Self-adjointness and invariance of the essential spectrum for the Klein–Gordon equation," *Helv. Phys. Acta* **50** (1977), 100–117, and "Scattering theory for the Klein–Gordon equation," *J. Functional Analysis* **27** (1978).

Section XI.16 The Haag–Ruelle theory is based on work of R. Haag, "Quantum field theories with composite particles and asymptotic completeness," *Phys. Rev.* **112** (1958), 669–673; "The framework of quantum field theory," *Nuovo Cimento Supp.* **14** (1959), 131–152; and D. Ruelle, "On the asymptotic condition in quantum field theory," *Helv. Phys. Acta* **35** (1962), 147–163. Haag presented the basic elements of the proof of Theorem XI.109 including the introduction of TVEV, and he postulated the falloff of these TVEV. He did not give a rigorous proof of the falloff of regular wave packets for the Klein–Gordon equation but based his proof on the correct bounds which were only proven formally. Ruelle supplied these two details essentially by proving Theorem XI.109 by the method used in this section and the corollary to Theorem XI.17 by a related but distinct method. Earlier, various authors had obtained partial results on clustering of TVEVs: G. Dell'Antonio and P. Gulmanelli, "Asymptotic conditions in quantum field theories," *Nuovo Cimento* **12** (1959), 38–53; H. Araki, "On the asymptotic behavior of vacuum expectation values at large space like separation," *Ann. Physics* **11** (1960), 260–274; and R. Jost and K. Hepp, "Über die Matrixelemente des Translation operators," *Helv. Phys. Acta* **35** (1962), 34–46. Theorem XI.111 is due to L. Schwartz in his book on distributions (see the notes to Sections V.3 and V.4).

There are "textbook" presentations of the Haag–Ruelle theory in various places: Jost's book quoted in the notes to Section IX.8; *Introduction to Axiomatic Quantum Field Theory* by N. N. Bogoliubov, A. A. Logunov, and I. T. Todorov, Benjamin, New York, 1975; and in K. Hepp, "On the connection between Wightman and LSZ quantum field theory," pp. 135–246 in *Axiomatic Field Theory: Brandeis University, 1965* (M. Chrêtien and S. Deser, eds.), Gordon and Breach, New York, 1966. All these treatments, as well as ours, follow Ruelle's approach.

If the function in Theorem XI.110 is in C_0^∞, then the falloff of $G(\alpha)$ is exponential; see H. Araki, K. Hepp, and D. Ruelle, "On the asymptotic behavior of Wightman functions in space-like directions," *Helv. Phys. Acta* **35** (1962), 164–174.

Lorentz covariance of scattering theory is a result of Ruelle (in the paper above) and is further discussed in the above textbook presentations. Ruelle also discusses the case of higher spin particles and fields. One critical aspect of this presentation is that odd (respectively, even) spin fields only produce odd (respectively, even) spin asymptotic fields. This is critical for the physical interpretation of the spin–statistics theorem. Haag and Ruelle also discuss what to do if property 10 fails—one uses suitable polynomials in the fields. A transcription of the Haag–Ruelle theory into the C^* algebraic approach to quantum field theory appears in R. Haag and H. Araki, "Collision cross sections in terms of local observables," *Comm. Math. Phys.* **4** (1967), 77–91.

Our physical interpretation of Theorem XI.109 as a scattering theory depended on rewriting it in the form of two Hilbert space wave operators (Corollary 2), but one can also justify its interpretation by rewriting N-body nonrelativistic quantum theory as a field theory and rewriting its scattering theory in a form analogous to Theorem XI.109. This has been done in W. Sandhas, "Definition and existence of multichannel scattering states," *Comm. Math. Phys.* **3** (1966), 358–374 and in Hepp's lectures (Hepp says he is following, in part, unpublished work of W. Hunziker); see also Problem 142.

Corollary 1 of Theorem XI.109 is related to a general result proven in the C^*-algebraic approach to relativistic quantum theory; namely that $\sigma(P_\mu)$ is additive; that is, if p_μ, $q_\mu \in \sigma(P_\mu)$, then $p_\mu + q_\mu \in \sigma(P_\mu)$. This was proven by H. J. Borchers, "Local rings and the connection of spin with statistics," *Comm. Math. Phys.* **1** (1965), 281-307.

If one restricts the regular wave packets $f^{(1)}, \ldots, f^{(n)}$ to have nonoverlapping velocities (that is, if $p_i \in \operatorname{supp} \hat{f}^{(i)}$ and $p_j \in \operatorname{supp} \hat{f}^{(j)}$ implies that $p_i/\mu(p_i) \neq p_j/\mu(p_j)$), then $\|d\eta/dt\|$ falls off faster than t^{-N} for any N rather than only like $t^{-3/2}$. This allows one to develop a Haag-Ruelle theory in two and three space-time dimensions and also allows one to avoid Theorem XI.110; these ideas are discussed in Hepp's lectures and in his paper "On the connection between LSZ and Wightman quantum field theory," *Comm. Math. Phys.* **1** (1965), 95-111.

There is an alternative asymptotic condition which is based on proving that *matrix elements* of the relativistic field $\int A(x)f(x, s-t)\, d^3x\, ds$ approach those of φ_{in} and φ_{out} smeared as $t \to \mp\infty$ (this is to be compared with the vector convergence of Theorem XI.109). Scattering theory based on these assumptions was developed by H. Lehmann, K. Symanzik, and W. Zimmerman, "Zur Formulierung Quantisierter Feldtheorien," *Nuovo Cimento* **1** (1955), 205-225 and "The formulation of quantized field theories, II," *Nuovo Cimento* **6** (1957), 319. This "LSZ theory" is further developed in V. Glaser, H. Lehmann, and W. Zimmerman, "Field operators and retarded functions," *Nuovo Cimento* **6** (1957), 1122-1128. Hepp in the above quoted paper and lecture notes proves that, in the Haag-Ruelle framework, matrix elements of suitable smoothed fields between states $\eta^{\text{in}}(f_1, \ldots, f_n)$ where the f's have nonoverlapping velocities converge to the same matrix elements of φ_{in} as $t \to -\infty$. The first really significant result in the LSZ formalism is an explicit formula for the S-matrix in terms of the Wightman distributions. These **reduction formulas** are proven for distinct velocities in Hepp's work. The reduction formulas are the first step in the analysis of the analyticity properties of scattering amplitudes in axiomatic field theory. Certain aspects of these developments together with extensive references can be found in A. Martin, *Scattering Theory: Unitarity, Analyticity, and Crossing*, Lecture Notes in Physics **3**, Springer-Verlag, New York, Heidelberg, Berlin, 1969.

Asymptotic completeness has not yet been verified in any of the models of interacting Wightman fields that have been constructed. It can sometimes happen that asymptotic completeness fails because one has not included enough fields. An artificial example is the following: Suppose that one could construct an interacting quantum electrodynamics that did have asymptotic completeness, and then one restricted the theory to the electromagnetic field and the cyclic subspace that it generates. This theory would not be asymptotically complete because the Hilbert space would contain two-particle electron–positron states without containing the corresponding one-particle states that are not coupled to the vacuum by the electromagnetic fields since they are charged. There is strong evidence that similar phenomena will take place in certain two-dimensional self-interacting Boson fields where it is believed that certain two-particle states (soliton and antisoliton pairs) are coupled to the vacuum by the Bose field even though the corresponding single particle states are not. See, J. Fröhlich, "New super-selection sectors ("soliton-states") in two dimensional bose quantum field models," *Comm. Math. Phys.* **47** (1976), 269-310; "Phase transitions, Goldstone bosons and topological superselection rules," Part 2, *Acta Phys. Austriaca, Suppl.* **XV** (1976), 133-269; "Quantum theory of non-linear invariant wave (field) equations. Or: Super selection sectors in constructive quantum field theory," in *Invariant Wave Equations* (G. Velo and A. S. Wightman, eds.), Springer Physics Lecture Notes *73*, 1978, and J. Bėllisard, J. Fröhlich, and B. Gidas, paper to appear in *Comm. Math. Phys.*

There has been considerable progress in the understanding of the weakly coupled $P(\varphi)_2$ theories in the energy region where no three-particle states occur, including a proof of "asymptotic completeness" for these energies. The basic papers are T. Spencer, "The decay of the

Bethe–Salpeter kernel in $P(\varphi)_2$ quantum field models," *Comm. Math. Phys.* **44** (1975), 143–164; T. Spencer and F. Zirilli, "Scattering states and bound states in $\lambda P(\varphi)_2$," *Comm. Math. Phys.* **49** (1975), 1–16. Further developments can be found in J. Glimm and A. Jaffe, "Two and three body equations in quantum field models," *Comm. Math. Phys.* **44** (1975), 293–320; and in J. Dimock and J.-P. Eckmann, "On the bound state in weakly coupled $\lambda(\varphi^6 - \varphi^4)_2$," *Comm. Math. Phys.* **51** (1976), 41–54; and "Spectral properties and bound state scattering for weakly coupled $\lambda P(\varphi)_2$ models," *Ann. Physics* **103** (1977), 289–314.

The TVEVs have analogues in probability theory where they are called **higher order cumulants** and in statistical mechanics where they are called **Ursell functions**. An elegant "axiomatic" characterization of Ursell functions and the resulting theory can be found in J. Percus, "Correlation inequalities for Ising spin lattices," *Comm. Math. Phys.* **40** (1975), 283–308. Among the significant results about TVEVs are an inversion formula (Problem 143), the relation to connectedness in diagrammatic expansions (Problem 144), and the following formula of P. Cartier, unpublished; see also the Percus paper quoted above and G. Sylvester, "Representations and inequalities for Ising model Ursell functions," *Comm. Math. Phys.* **42** (1975), 209–220:

$$(\psi_0, \varphi(x_1) \cdots \varphi(x_n)\psi_0)_T = \frac{1}{n}(\Psi_0, \Phi(x_1) \cdots \Phi(x_n)\Psi_0) \tag{349a}$$

$$\Phi(x_i) = \sum_{j=1}^{n} \omega^j \varphi_j(x_i) \tag{349b}$$

In (349b), ω is a primitive nth root of unity (that is, $\omega^n = 1, \omega^j \neq 1, j = 1, \ldots, n-1$) and $\varphi_1, \ldots, \varphi_n$ are independent copies of φ; that is, we take $\mathscr{H}' = \mathscr{H} \otimes \cdots \otimes \mathscr{H}$ (n times), $\Psi_0 = \psi_0 \otimes \cdots \otimes \psi_0$ and

$$\varphi_j(x) = 1 \otimes \cdots \otimes \varphi(x) \otimes \cdots \otimes 1 \qquad (j\text{th place})$$

Scattering theory for massless particles in an axiomatic (C^*-algebraic) framework has been developed in two remarkable papers by D. Buchholz, "Collision theory for massless fermions," *Comm. Math. Phys.* **42** (1975), 269–279; and "Collision theory for massless bosons," *Comm. Math. Phys.* **52** (1977), 147–173. While Buchholz uses some parts of the Haag–Ruelle theory, temperedness of the TVEV does not hold, so very different ideas are needed. In fact, the key idea is to exploit the fact that solutions of the wave equation obey Huygens' principle. For this reason, once the limit of $A_f(t)\Omega_0$ (suitably defined) is controlled (this is not independent of time because one cannot separate the one-particle zero mass states from the continuum), one can control the limit of $A_f(t)F\Omega_0$ for any F obtained by smearing fields with functions supported in suitable sets (basically the "hole" obtained by excluding the union of the boundaries of the light cones with vertex at points in supp $f(x, t = 0)$). In this way one obtains the existence of $\lim A_f(t)\psi$ for a dense set of ψ.

It is to be emphasized that when massless particles are present, one does not know how to construct scattering states for the *massive* particles. In fact, it is not clear how to "separate" the massive particle from the massless ones—it may be that in a theory of electrons and photons there is no discrete piece of the mass spectrum corresponding to one electron but that somehow only electrons accompanied by infinitely many low energy photons occur—this problem which is not completely understood, is called the **infrared problem**. There is an exhaustive literature on this subject beginning with F. Bloch and A. Nordsieck, "A note on the radiation field of the electron," *Phys. Rev.* **52** (1937), 54–59; and D. Yennie, S. Frautschi, and H. Suura, "The infrared divergence phenomena and high-energy processes," *Ann. Physics* **13** (1961), 379–452. For a discussion of more recent literature, see J. Fröhlich, "On the infrared problem in a model of scalar electrons and massless, scalar bosons," *Ann. Inst. H. Poincaré Sect. A* 19 (1973), 1–103. It should also be mentioned that this same phenomenon could occur with the massless particles, in which case Buchholz's theory would not apply since he assumes that states with $H^2 - \mathbf{P}^2 = 0$ $(H \neq 0)$ occur.

Section XI.17 The discussion in this section is based primarily on the beautiful paper of V. Enss, "Asymptotic completeness for quantum mechanical potential scattering," *Comm. Math. Phys.*, to appear. We use some technical devices borrowed from B. Simon, "Phase space analysis of simple scattering systems: Extensions of some work of V. Enss," *Duke Math. J.*, to appear. This latter paper extends the theory to allow H_0 to be replaced by a wide variety of differential and pseudo-differential operators including Dirac Hamiltonians. Enss has extended the method to include Coulomb potentials and has presented a program, which he is currently implementing, to handle multiparticle scattering.

Wiener's theorem (Theorem XI.114) was proven by N. Wiener in his book *The Fourier Integral and Certain of Its Applications*, Cambridge University Press, London, 1935. Its consequences (including the corollary to Theorem XI.115) have been used in ergodic theory for many years; see especially, Section 8 of K. Jacobs, *Lecture Notes on Ergodic Theory*, Aarhus Lecture Note Series 1 (1962/63).

The importance of Wiener's theorem for geometrically characterizing the continuous spectrum in scattering problems was discovered independently by Lax–Phillips–de Leeuw (see p. 145 in the book of Lax and Phillips quoted in the notes to Section 11) and by D. Ruelle, "A remark on bound states in potential scattering theory," *Nuovo Cimento A* 61 (1969), 655–662. Lax–Phillips use Wiener's theorem to prove directly the corollary to Theorem XI.115 and they then use that to establish (219). Ruelle proved for a large class of Schrödinger operators including multiparticle ones that, for all R,

$$\frac{1}{2T}\int_{-T}^{T} \|F(|x| \leq R)e^{-itH}\varphi\|^2\, dt \to 0$$

as $T \to \infty$ if and only if $\varphi \in P_{\text{cont}}(H)$. W. Amrein and V. Georgescu in "Bound states and scattering states in quantum mechanics," *Helv. Phys. Acta* 46 (1973), 633–658, extended Ruelle's results and, in particular, realized that the compactness of $F(|x| \leq R)(H + i)^{-1}$ was the critical factor (this was disguised in Ruelle's discussion). None of these authors noted the uniformity in φ (one can use Wiener's theorem directly to show that $(\psi, e^{-itA}\varphi)$ goes to zero in L^2 mean if ψ is in $\mathscr{H}_{\text{cont}}$); the stated uniformity is an unpublished remark of Enss.

The final theorem in the appendix is due to V. Enss.

NOTES ON SCATTERING THEORY ON C^*-ALGEBRAS

There is a simple generalization of scattering theory ideas to the framework of C^*-algebras. In these notes we shall discuss some of the more interesting aspects of these ideas using freely the terminology of C^*-algebras. This discussion should be supplemented with the explicit examples to be found in the references below.

First, we want to discuss the relation of scattering theory to the approach to equilibrium in statistical mechanics. As a starting point, let H_0 be a self-adjoint operator on a Hilbert space $\mathscr{H}$

and let V be in $\mathscr{L}(\mathscr{H})$. Consider the natural automorphisms on $\mathscr{L}(\mathscr{H})$: $\alpha_t^{(0)}(A) = e^{iH_0t}Ae^{-iH_0t}$ and $\alpha_t(A) = e^{iHt}Ae^{-iHt}$ where $H = H_0 + V$. Let $\beta_t = \alpha_t\alpha_{-t}^{(0)}$. Then

$$\frac{d}{dt}\beta_t(A) = i\beta_t(\alpha_t^{(0)}[V, \alpha_{-t}^{(0)}(A)]) = i\beta_t([\alpha_t^{(0)}(V), A])$$

or

$$\beta_t(A) = A + i\int_0^t \beta_s([\alpha_s^{(0)}(V), A])\, ds \tag{350}$$

(350) can be solved by iteration:

$$\beta_t(A) = A + \sum_{n=1}^{\infty} \beta_t^{(n)}(A) \tag{351}$$

with

$$\beta_t^{(n)}(A) = (i)^n \int_0^t \int_0^{s_1} \int_0^{s_2} \cdots \int_0^{s_{n-1}} [\alpha_{s_n}^{(0)}(V), [\alpha_{s_{n-1}}^{(0)}(V), \ldots [\alpha_{s_1}^{(0)}(V), A] \cdots]]\, ds_n\, ds_{n-1} \cdots$$

A simple estimate shows that $\|\beta_t^{(n)}(A)\| \le 2^n(t^n/n!)\|V\|^n\|A\|$, so the series (351) converges to a solution of (350). Equivalently:

$$\alpha_t(A) = \alpha_t^{(0)}(A) + \sum_{n=1}^{\infty} (i)^n \int_{0 \le s_n \le \cdots \le s_1 \le t} [\alpha_{s_n}^{(0)}(V), [\cdots, [\alpha_{s_1}^{(0)}(V), \alpha_t^{(0)}(A)] \cdots]\, ds_1 \cdots ds_n \tag{352}$$

(352), which expresses α_t in terms of only $\alpha_t^{(0)}$ and V, is the starting point for a general theory of perturbations of automorphisms of C^*-algebras. For suppose that $\alpha_t^{(0)}$ is a norm-continuous one-parameter group of automorphisms of a C^*-algebra $\mathfrak{A}$ and let $V \in \mathfrak{A}$. The expression in (352) converges to a norm-continuous one-parameter group of automorphisms which we denote by α_t. It is now fairly easy to prove (see Problem 147):

Theorem XI.117 Let π be a representation of a C^*-algebra $\mathfrak{A}$ on a Hilbert space $\mathscr{H}$ and let $\alpha_t^{(0)}$ and α_t be as above. Suppose that there is a one-parameter strongly continuous unitary group U_t on $\mathscr{H}$ with

$$\pi(\alpha_t^{(0)}(A)) = U_t\pi(A)U_{-t} \tag{353a}$$

Let H_0 be the infinitesimal generator of U_t and let $W_t = e^{i(H_0+\pi(V))t}$. Then

$$\pi(\alpha_t(A)) = W_t\pi(A)W_{-t} \tag{353b}$$

Conversely, if (353b) holds for some W_t, then (353a) holds for some U_t.

Thus, we see that $\alpha_t^{(0)}$ and α_t are unitarily implementable in precisely the same representations.

Now one seeks to control $\lim_{t\to\mp\infty} \alpha_{-t}\alpha_t^{(0)}(A)$. (352) and Cook's method (Section 3) immediately imply:

Theorem XI.118 Suppose that for a dense subspace $\mathfrak{A}_0 \subset \mathfrak{A}$ and all $A \in \mathfrak{A}_0$,

$$\|[\alpha_{(\cdot)}^{(0)}(V), A]\| \in L^1(\cdot) \tag{354}$$

Then for any $A \in \mathfrak{A}$, $\lim_{t\to\pm\infty} \alpha_{-t}\alpha_t^{(0)}(A)$ exist and $w^\pm = \text{s-}\lim_{t\to\mp\infty} \alpha_{-t}\alpha_t^{(0)}$ are injective morphisms on $\mathfrak{A}$ obeying

$$w^\pm(\alpha_s^{(0)}(A)) = \alpha_s(w^\pm(A)) \tag{355}$$

D. Robinson has suggested a very beautiful connection between Theorem XI.118 and the approach to equilibrium in quantum lattice gases: Let $\alpha_t^{(0)}$ be the time translations in a lattice gas. Let V be a local observable. Then, if A is a local observable, (354) is to be expected (and can be proven in some models!) since as $t \to \pm\infty$, $\alpha_t^{(0)}(V)$ is "spread out" over a larger and larger region. Let φ be an invariant state for α_t, that is, for the locally perturbed dynamics. Then $\varphi(\alpha_t^{(0)}(\cdot)) = \varphi(\alpha_{-t}\alpha_t^{(0)}(\cdot)) \to \varphi(w^\pm(\cdot))$ and, by (355), $\varphi(w^\pm(\cdot))$ are invariant states for $\alpha_t^{(0)}$. Thus, if φ moves according to the free dynamics, it approaches an invariant state for $\alpha_t^{(0)}$. Moreover, under some additional hypotheses, if φ is a KMS state for α_t at temperature T, then $\varphi(w^\pm(\cdot))$ are KMS states for $\alpha_t^{(0)}$ at temperature T.

This example of C^*-algebra scattering theory and its relation to statistical mechanics is due to D. Robinson, "Return to equilibrium," *Comm. Math. Phys.* **31** (1973), 171–189. Robinson's paper contains the details of the theorems discussed above and calculations in some explicit models. Some aspects of the C^*-algebra approach to scattering used by Robinson already appeared in R. F. Streater, "On certain non-relativistic quantized fields," *Comm. Math. Phys.* **7** (1968), 93–98; and K. Hepp, "Rigorous results on the s-d model of the Kondo effect," *Solid State Comm.* **8** (1970), 2087–2090. For additional discussion of approach to equilibrium in statistical mechanics (from a nonscattering point of view), see C. Radin, "Gentle perturbations," *Comm. Math. Phys.* **23** (1971), 189–198; O. Lanford, III and D. Robinson, "Approach to equilibrium of free quantum systems," *Comm. Math. Phys.* **24** (1972), 193–210.

In many cases (354) is too strong and $\alpha_{-t}\alpha_t^{(0)}$ is not norm convergent but only weakly convergent. In such cases it is more natural to suppose that $\mathfrak{A}$ is a von Neumann algebra. An approach of this sort is used in some studies of long-range potential scattering. Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^n)$. Let $\mathfrak{A} = \{H_0\}'$, the family of operators commuting with bounded functions of H_0. Let V be a long-range potential of the sort for which modified wave operators exist. Let $\alpha_t(A) = e^{iHt}Ae^{-iHt}$ (which may not be in $\mathfrak{A}$ but only in $\mathcal{L}(\mathcal{H})$). Then

$$\operatorname*{w-lim}_{t \to \mp\infty} \alpha_t(A) = \operatorname*{w-lim}_{t \to \mp\infty} e^{iHt}U_D(-t)AU_D(t)e^{-iHt} = \Omega_D^\pm A(\Omega_D^\pm)^*$$

References for the C^*-algebra approach to long-range scattering can be found in the notes to Section 9.

Scattering in terms of automorphisms also plays a role in the study of spectral properties of Hamiltonians in certain cutoff quantum field theory models. Let us indicate the general ideas in the application to the cutoff $P(\varphi)_2$ field theory. Let $a_t^*(f) = e^{iHt}e^{-iH_0t}a^*(f)e^{iH_0t}e^{-iHt}$. Formally,

$$\frac{d}{dt}a_t^*(f) = ie^{iHt}[V, e^{-iH_0t}a^*(f)e^{iH_0t}]e^{-iHt}$$

This formula, the Cook method, and certain estimates of L. Rosen, "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457, allow one to prove that $\lim_{t\to\mp\infty} a_t^*(f)\psi$ exist for a family of f's dense in the one-particle space and ψ's dense in Fock space. The limiting operators $a_\pm^*(f)$ can be shown to have three important additional properties: (1) $[a_\pm^\dagger(f), a_\pm(g)] = -(Cf, g)$; enough control on the limit allows one to prove that the algebraic relations are preserved. (2) Since e^{iH_0t} is of the special form $e^{iH_0t} = \Gamma(e^{i\omega t})$ for a one-particle operator ω, the intertwining relations take the form $e^{iHt}a_\pm^*(f)e^{-iHt} = a_\pm^*(e^{i\omega t}f)$. (3) If ψ is an eigenvector of H, then $a_\pm(f)\psi = 0$ for all f. This follows from the fact that $\operatorname{s-lim}_{t\to\pm\infty} a(e^{i\omega t}f)N^{-1/2} = 0$ and Rosen's estimates. (1) and (3) allow one to build up a subspace $\mathcal{H}_\psi \subset \mathcal{H}$ and a Fock representation for $a_\pm^*(f)$ with ψ as vacuum for any eigenvector ψ of H. Since it is known that there is a vector with $H\psi = E_0\psi$ (see Section XIII.12), (2) and this construction imply that $H \restriction \mathcal{H}_\psi$ is unitarily equivalent to $H_0 + E_0$ from which it follows that $[m_0 + E_0, \infty) \subset \sigma_{\text{ac}}(H)$.

The idea of using scattering theory to study quantum field Hamiltonians via the construction of asymptotic creation and annihilation operators $a_{\pm}^{*}$ was first presented in Y. Kato and N. Mugibayashi, "Regular perturbations and asymptotic limits of operators in quantum field theory," *Progr. Theoret. Phys.* **30** (1963), 103–133; and developed in a series of papers by R. Höegh-Krohn, "Asymptotic limits in some models of quantum field theory, I, II, III," *J. Mathematical Phys.* **9** (1968), 2075–2080; **10** (1969), 639–643; **11** (1970), 185–188; and "On the scattering operator for quantum fields," *Comm. Math. Phys.* **18** (1970), 109–126. The theory was used to study spectral properties of spatially cutoff $P(\varphi)_2$ Hamiltonians (see Sections X.7 and X.9) by R. Höegh-Krohn, "On the spectrum of the space cutoff $:P(\varphi):$ Hamiltonian in two space-time dimensions," *Comm. Math. Phys.* **21** (1971), 256–260; and Y. Kato and N. Mugibayashi, "Asymptotic fields in the $\lambda(\varphi^4)_2$ quantum field theory," *Progr. Theoret. Phys.* **45** (1971), 628–639; and for the Y_2 field theory by J. Dimock, "Spectrum of local Hamiltonians in the Yukawa$_2$ field theory," *J. Mathematical Phys.* **13** (1972), 477–481. In either case, one proves that $[m_0 + E_0, \infty) \subset \sigma_{ac}(H)$ where $E_0 = \inf \sigma(H)$ and m_0 is the free mass in H_0. Since one knows that $\sigma_{ess}(H) \subset [m_0 + E_0, \infty)$ by results of J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory without cutoffs, II: The field operators and the approximate vacuum," *Ann. of Math.* **91** (1970), 362–401, (for $(\varphi^4)_2$) and "Self-adjointness of the Yukawa$_2$ Hamiltonian," *Ann. Physics* **60** (1970), 321–383 (for Y_2); and of L. Rosen "A $\lambda\varphi^{2n}$ field theory with cutoffs," *Comm. Math. Phys.* **16** (1970), 157–183 (for $P(\varphi)_2$); one can conclude that $\sigma_{ac}(H) = \sigma_{ess}(H) = [m_0 + E_0, \infty)$ for these models. We remark that the methods of Kato–Mugibayashi and Höegh-Krohn are restricted to models for which there is no renormalization of Hilbert space. For realistic field theories, one must fall back on the Haag–Ruelle theory of Section 16.

PROBLEMS

†*1*. Under hypotheses (3), prove that for any $\langle r_0, v_0 \rangle \in \mathbb{R}^6$, there is a solution of (2) for all time. (*Hint*: Consult the discussion of classical motion on the real line in the appendix to Section X.1.)

2. Prove that if (4a) holds, but not necessarily (4b), then the map constructed in the proof of Theorem XI.1 has at least one fixed point.

3. Find an example of a force F for which (4a) holds, where (4b) is false, and where the map in Theorem XI.1 has more than one fixed point, that is, where scattering states exist but are not unique.

Reference for Problems 2, 3: The paper of Simon quoted in the notes to Section XI.2.

†*4*. Prove that under the hypothesis that F obeys (4), the integral equation (6) is equivalent to the differential equation (2a) with boundary conditions (5).

†*5*. Let $\mathcal{M}$ be a complete metric space and let $c < 1$.
  (a) Let $\{F_n\}$, F_∞ be a family of maps on M obeying $\rho(F_n x, F_n y) \le c\rho(x, y)$ for all n and all $x, y \in \mathcal{M}$. Suppose that $F_\infty x = \lim_{n\to\infty} F_n x$ for all x and that $F_n x_n = x_n$, $F_\infty x_\infty = x_\infty$. Prove that $x_n \to x_\infty$.
  (b) Let $F: \mathbb{R} \times \mathcal{M} \to \mathcal{M}$ be continuous and obey $\rho(F(t, x), F(t, y)) \le c\rho(x, y)$ where $c < 1$. Suppose that $\mathcal{M}$ is a subset of a Banach space and that $F(t, x)$ is C^∞ jointly

in x and t as a map from $\mathbb{R} \times \mathcal{M}$ into $\mathcal{M}$ (differentiable in the Fréchet sense). Define $g(t) \in \mathcal{M}$ by $F(t, g(t)) = g(t)$. Prove that $g(t)$ is a C^∞ vector-valued function.

†6. Complete the proof of Theorem XI.2a.

†7. Prove that under the hypotheses of Theorem XI.2, the map $\mathcal{F}_{a,b}^{(-\infty)}: \Sigma_0 \times \mathcal{M}_T \to \mathcal{M}_T$ obeys all the hypotheses of Problem 5b with the obvious modification necessary when $\mathbb{R}$ is replaced by a subset of $\mathbb{R}^6$.

*8. Develop scattering theory in n-body classical systems in the scattering channel where all particles are asymptotically free. Consider the problems that arise in attempting the extension to channels with some bound states.

9. Find a central force and a solution of Newton's equation in that force field for which $\lim_{t\to-\infty} |r(t)| = \infty$; $\lim_{t\to+\infty} |r(t)| = r_0 < \infty$.

†10. Prove that the sets $\Sigma_{\text{bound}}, \Sigma_0, N_\pm, N_\pm^{(n)}, \Sigma'$ used in the proof of Theorem XII.3 are all measurable.

11. Prove formulas (7a) and (7b) for the functions $\theta(E, \ell)$ and $T(E, \ell)$ in a central force field. *Reference:* Newton's book quoted in the notes to Section 2.

12. Verify the formula for $d\sigma/d\Omega$ in the central case.

13. Consider the statement: Total cross sections are usually infinite in classical mechanics.

14. In the context of Theorem XI.3 but with the additional hypothesis that $V(\mathbf{r})$ is a central potential, find an alternative proof that if $E > 0$ and $\overline{\lim}_{t\to\infty} |r(t)| = \infty$, then $\lim_{t\to\infty} |r(t)|t^{-1} > 0$. (*Hint:* Use conservation of energy and angular momentum.)

15. (a) Let A be a self-adjoint operator. Prove that $e^{i(A-\lambda)t}\varphi$ has a norm limit as $t \to \infty$ if and only if φ is an eigenvector of A with eigenvalue λ. (*Hint:* Compute the weak limit of $T^{-1} \int_0^T e^{i(A-\lambda)t}\varphi \, dt$.)
    (b) Let A and B be self-adjoint. Prove that $e^{iAt}e^{-iBt}$ converges in operator norm as $t \to \pm\infty$ if and only if $A = B$.

16. Let H_0 be a fixed operator and let V_n and V_∞ be H_0-bounded operators with relative bound a less than 1, so that $H_0 + V_n \to H_0 + V_\infty$ in strong resolvent sense. Suppose that there is a dense set, D in $P_{\text{ac}}(H_0)$ so that for $u \in D$: $\sup_{n\le\infty} \|V_n e^{-itH_0}u\| \equiv f_u(t)$ is in $L^1(\mathbb{R})$. Prove that $\Omega^\pm(H_0 + V_n, H_0)$ converge strongly to $\Omega^\pm(H_0 + V, H_0)$. (*Hint:* First show that $\Omega(H_0 + V_n, H_0)u = u + i\int_0^\infty e^{i(H_0+V_n)t}V_n e^{-itH_0}u$ and then use dominated convergence.) *Reference:* The paper of Davies quoted in the notes to Section 4.

†17. (a) Show that $|||\cdot|||$ is a norm on $\mathcal{M}(B)$. Is $\mathcal{M}(B)$ complete in this norm? (*Hint:* Use (16).)
    (b) Show that $\mathcal{M}(B)$ is dense in $P_{\text{ac}}(B)$ in the usual norm.

18. Let C be a bounded operator with $C(A+i)^{-n}$ compact for some n where A is self-adjoint. Prove that $Ce^{-iAt}P_{\text{ac}}(A) \to 0$ strongly as $t \to \pm\infty$. Prove the same thing if $CE_I(A)$ is compact for all bounded intervals I.

19. Prove Theorem XI.5 by first showing that s-lim $e^{iAt}(1-\chi)e^{-iBt}$ exist and then, using Problem 18, that s-lim $\chi e^{-iBt} = 0$.

20. Let A and B be self-adjoint operators with $Q(A) = Q(B)$. Let $\varphi, \psi \in Q(A)$. Prove that $(\varphi, e^{iAt}e^{-iBt}\psi)$ is differentiable with derivative $i(\varphi, e^{iAt}(A - B)e^{-iBt}\psi)$ and verify (15).

†21. Fill in the domain details in the proof of Pearson's theorem (Theorem XI.7).

22. Construct operators A_n and A so that $\|A_n - A\|_1 \to 0$, so that A_n has purely absolutely continuous spectrum $[0, 1]$, and so that A has absolutely continuous spectrum $[0, 1]$ and an eigenvalue at $\lambda = 0$. Conclude that $\Omega^\pm(A, A_n)$ cannot converge strongly to $\Omega^\pm(A, A)$.

23. Let $(A_n + i)^{-1} \to (A + i)^{-1}$ in trace class norm. Let $J_n = (A_n + i)^{-1}(A + i)^{-1}$ and $J = (A + i)^{-2}$. Prove that $\Omega^\pm(A_n, A; J_n) \to \Omega^\pm(A, A; J)$ strongly and conclude that $\Omega^\pm(A_n, A) \to P_{ac}(A)$. *Hint:* Use the fact that

$$\Omega^\pm(A_n, A; J_n)(A + i)^2 = \Omega^\pm(A_n, A)$$

Prove that $\Omega^\pm(A, A_n)P_{ac}(A) \to P_{ac}(A)$ strongly.

24. Suppose that $E_I(A_n)(A_n - A)E_I(A)$ goes to zero in trace class norm for each bounded interval I. Suppose, moreover, that the A_n are uniformly subordinate to A, that is, the functions involved in the definition of subordinate can be chosen to be independent of n. Prove that $\Omega^\pm(A_n, A) \to P_{ac}(A)$ and $\Omega^\pm(A, A_n)P_{ac}(A) \to P_{ac}(A)$ strongly.

25. Suppose that A and B are self-adjoint operators with $(A - z)^{-n} - (B - z)^{-n}$ trace class for all $\operatorname{Im} z \neq 0$.
    (a) Prove that $(A + i)^{-k} - (B + i)^{-k}$ is compact for any integer $k > n$. (*Hint:* Take derivatives by using the Cauchy integral formula.)
    (b) Let $J = \sum_{j=1}^{n} (A + i)^{-j}(B + i)^{-n+j-1}$. Use Pearson's theorem to prove that $\Omega^\pm(A, B; J)$ exist.
    (c) Let $J' = (A + i)^{-n+1}J$. Prove that $\Omega^\pm(A, B; J')$ exist.
    (d) Let $J'' = (B + i)^{-2n}$. Prove that $\Omega^\pm(A, B; J'')$ exist and equal $n\Omega^\pm(A, B; J')$. (*Hint:* Use (a).)
    (e) Prove that $\Omega^\pm(A, B)$ exist and are complete.

†26. Prove part (a) of Lemma 3 used in the Kato–Birman theory.

27. Let A and B be self-adjoint operators. Prove that $(A - z)^{-1} - (B - z)^{-1}$ is trace class for some $z \in \rho(A) \cap \rho(B)$ if and only if it is trace class for all $z \in \rho(A) \cap \rho(B)$.

28. Let $A_n \to A$ in trace class norm. Let φ be an admissible function. Prove that $\Omega^\pm(\varphi(A_n), \varphi(A)) \to P_{ac}(A)$ and $\Omega^\pm(\varphi(A), \varphi(A_n))P_{ac}(A) \to P_{ac}(A)$ strongly as $n \to \infty$.

29. (a) Let $F(z) = (A + E)^{-z-\frac{1}{2}}C(B + E)^{-k(1-z)-\frac{1}{2}}$. Suppose that $F(0)$ and $F(1)$ are trace class. Prove that $F(z)$ is trace class for all z with $0 \leq \operatorname{Re} z \leq 1$. (*Hint:* Apply the three lines lemma to $\operatorname{Tr}(F(z)K)$ for finite rank K.)
    (b) Prove (36).

30. Prove Proposition 5 of Section 3.

31. (a) Let $A = -d^2/dx^2$ on $L^2(0, \infty)$ with $u(0) = 0$ boundary conditions. Let $B = A + V$ defined as a sum of quadratic forms where $V \in L^1_{loc}(0, \infty)$ is positive (V may have arbitrarily bad growth at $r = 0$) and supp $V \subset [0, 1]$. Let $\tilde{A} = -d^2/dx^2$ on $L^2(0, 1) \oplus L^2(1, \infty)$ with $u(0) = u(1) = 0$ boundary conditions on the first factor and $u(1) = 0$ boundary conditions on the second. Let $\tilde{B} = \tilde{A} + V$. Prove that $(\tilde{A} + 1)^{-1} - (A + 1)^{-1}$ and $(\tilde{B} + 1)^{-1} - (B + 1)^{-1}$ are trace class (*Hint:* They are finite rank.)

(b) Let $\tilde{A} = A_1 \oplus A_2$. Prove that $(A_1 + 1)^{-1}$ and $(B_1 + 1)^{-1}$ are trace class and conclude that $(\tilde{A} + 1)^{-1} - (\tilde{B} + 1)^{-1}$ is trace class.

(c) Prove that $(A + 1)^{-1} - (B + 1)^{-1}$ is trace class.

*(d) Extend these ideas to n dimensions. (*Hint*: See the paper of Deift and Simon quoted in the notes to Section 4.)

32. (a) Given an operator A on a Hilbert space $\mathscr{H}$ that is not densely defined but with A self-adjoint on $D(A)$, define e^{iAt} and $(A + i)^{-1}$ on $\mathscr{H}$ by setting them to zero on $D(A)^\perp$. Extend the Kuroda–Birman theorem to this setting.

(b) Let $B = -\Delta$ on $L^2(\mathbb{R}^n)$ and A be the operator on $L^2(\mathbb{R}^n \backslash \{x \mid |x| < 1\})$ with Dirichlet boundary conditions on the sphere. Prove that the Kuroda–Birman theorem in the extended form (a), with $(A + i)^{-n}$ replacing $(A + i)^{-1}$, is applicable. Is Birman's theorem applicable?

(c) Use these ideas to discuss obstacle scattering (Section 10) without the trick of adding dynamics to the interior.

*†*33.* (a) Prove Theorem XI.19a by using finite propagation speed.

(b) Let $\varphi(x, t)$ solve the wave equation with initial data in $\mathscr{S}(\mathbb{R}^n)$. Let $x = \langle x_1, 0, \ldots, 0\rangle$ with $x_1 > 0$. Prove that $\varphi(x, t) = \varphi_+(x, t) + \varphi_-(x, t)$ with

$$\varphi_\pm(x, t) = \int_{S^{n-1}} d\Omega \int_0^\infty \alpha^{n-2} e^{i\alpha(\pm t + x_1 \cos\theta)} f_\pm(\alpha, \Omega)\, d\alpha$$

with $f_\pm$ smooth on $(0, \infty) \times S^{n-1}$ and continuous up to $\alpha = 0$.

(c) Prove that

$$\varphi_\pm(x, t) = \int_{S^{n-1}} g_\pm(\pm t + x_1 \cos\theta, \Omega)\, d\Omega$$

where $|g_\pm(y, \Omega)| \le C(1 + |y|)^{-(n-1)}$ and conclude that Theorem XI.19b holds.

(d) Make a stationary phase analysis in the $d\Omega$ variables to analyze the behavior if $|x|/t \in (1 - \varepsilon, 1 + \varepsilon)$ and complete the proof of Theorem XI.19c.

34. Apply stationary phase methods to time-dependent scattering theory.

†*35.* Fill in the details of the interpolation argument needed in the proof of Theorem XI.20.

36. Let $f(y) = e^{-y^2}$. Suppose that g is not in $L^2_{\text{loc}}(\mathbb{R}^n)$. Prove that $g(x)f(-i\nabla)$ is *not* a bounded operator and conclude that Theorem XI.20 does not extend to L^q for $q < 2$.

37. Let $\|f\|_{BS} = \sum_{m \in \mathbb{Z}^n} (\int_{0 \le x_i - m_i < 1} |f(x)|^2\, dx)^{1/2}$. Prove that if f and g satisfy $\|f\|_{BS} + \|g\|_{BS} < \infty$, then $f(x)g(i\nabla)$ is trace class and

$$\|f(x)g(-i\nabla)\|_1 \le c\|f\|_{BS}\|g\|_{BS}$$

(*Hint*: Use Theorem XI.21 to prove that $\|f(x)g(i\nabla)\|_1 \le c\|f\|_2\|g\|_2$ for any f and g each with support in some unit cube.)

Remark: The $\|\cdot\|_{BS}$ norm was used by Birman and Solomjak in their paper quoted in the notes to Section 3.

38. Suppose that $(1 + x^2)^{\delta/2}f(x)$ and $(1 + x^2)^{\delta/2}g(x)$ lie in $L^p(\mathbb{R}^n)$ where $2 \le p < \infty$ and $\delta > n/p$. Prove that $f(x)g(-i\nabla)$ is in $\mathscr{I}_{p/2}$. (*Hint*: Interpolate from Theorem XI.21.)

39. Suppose that $\Omega^{\pm}(A, B)$ exist.
    (a) Prove that $(1 - P_{[a,b]}(A))\Omega^{\pm}(A, B)P_{[a,b]}(B) = 0$.
    (b) Let $\varphi(x) = \alpha x + \beta$ for $x \in [a, b]$. Prove that:

$$\Omega^{\pm}(\varphi(A), \varphi(B))P_{[a,b]}(B) = \begin{cases} \Omega^{\pm}(A, B)P_{[a,b]}(B), & \alpha > 0 \\ \Omega^{\mp}(A, B)P_{[a,b]}(B), & \alpha < 0 \end{cases}$$

    (c) Prove an invariance principle for piecewise linear φ.

40. Under the coordinate change $R = (\mu_1 + \mu_2)^{-1}(\mu_1 r_1 + \mu_2 r_2)$, $r = r_2 - r_1$, show that $H = -(2\mu_1)^{-1}\Delta_1 - (2\mu_2)^{-1}\Delta_2 + V(r_1 - r_2)$ becomes

$$H = -(2M)^{-1}\Delta_R - (2m)^{-1}\Delta_r + V(r)$$

in the passive interpretation where $M = \mu_1 + \mu_2$ and $m^{-1} = \mu_1^{-1} + \mu_2^{-1}$.

41. Suppose that S is an $N \times N$ matrix and consider the coordinate change $x_i = \sum s_{ij} y_j$ on $\mathbb{R}^{3N}$. Suppose that $\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_{x_i}$ is transformed to $\sum_{i=1}^{N} (2\mu_i)^{-1}\Delta_{y_i}$ and that for all i and j, $x_i - x_j = \sum_{k=1}^{N-1} a_{ijk} y_k$ (note the $N - 1$). Prove that $y_N = a \sum_{i=1}^{N} \mu_i x_i$ where $a = (\sum_{i=1}^{N} \mu_i)^{-1/2}\mu_N^{-1/2}$.

†42. Prove (56) from (55).

†43. Prove that the linear combinations of the translates of $\varphi_\gamma(x) = \gamma^{-\frac{3}{2}}e^{-\frac{1}{2}\gamma x^2}$ are dense in $L^2(\mathbb{R}^3)$. (*Hint:* Obtain Hermite functions by taking derivatives.)

44. Suppose that $\int (1 + |y|)^{\alpha} |V(y)|^2 \, d^n y < \infty$ for some α with $n + \alpha > 2$. Prove that (45) holds, and conclude that $\Omega^{\pm}(-\Delta + V, -\Delta)$ exist. *Remark:* This result, unlike Theorem XI.24, holds in the case $n = 1, 2$.

45. Suppose that $V_t(x)$ is a family of functions with support in a fixed compact region whose L^2 norms are bounded by some power of t. Use stationary phase methods to prove that the time-dependent wave operators exist.

46. Suppose that A is a positive self-adjoint operator and B is a self-adjoint operator with:
    (i) $|B|$ is A-form bounded with relative bound $\alpha < 1$.
    (ii) $|B|^{1/2}(A + i)^{-1}$ is trace class.

    Prove that $(A + B + E)^{-1} - (A + E)^{-1}$ is trace class for E sufficiently large. (*Hint:* Let $B^{1/2} = B/|B|^{1/2}$ and use the formula

$$\begin{aligned}(A + B + E)^{-1} &- (A + E)^{-1} \\ &= -(A + E)^{-1}B^{1/2}(1 + |B|^{1/2}(A + E)^{-1}B^{1/2})^{-1}|B|^{1/2}(A + E)^{-1}.)\end{aligned}$$

47. (a) Prove that the kernel of $[-d^2/dx^2 + 1]^{-1}$ on $L^2(\mathbb{R})$ is $\frac{1}{2}e^{-|x-y|}$. (*Hint:* Use the Fourier transform.)
    (b) Let h_0 be the operator $-d^2/dx^2$ on $L^2(0, \infty)$ with zero boundary conditions at the origin. Prove that the kernel of $(h_0 + 1)^{-1}$ is $\frac{1}{2}e^{-|x-y|} - \frac{1}{2}e^{-(x+y)} = K(x, y)$. (*Hint:* Prove that $\int K(x, y)f(y)\, dy$ is in $D(h_0)$ and that $h_0 + 1$ applied to it is f.)

48. (a) Let V be in L^∞ with compact support. Knowing (63) for continuous V_n, prove it for V.
    (b) For arbitrary V, let V_n be in L^∞ with compact support and $V_n \uparrow |V|$ pointwise. Prove (63) for V.

†49. Prove the proposition preceding Theorem XI.33 concerning properties of the S-operator in two-body systems.

50. Let A be a positive self-adjoint operator and let B_∞ and B_n be self-adjoint operators, so that:

(i) $|B_n| \leq \frac{1}{2}A + c$ for some fixed c and all n.
(ii) $|B_n|^{1/2}(A+i)^{-1} \to |B_\infty|^{1/2}(A+i)^{-1}$ in Hilbert–Schmidt norm.
(iii) $[B_n/|B_n|^{1/2}](A+i)^{-1} \to [B_\infty/|B_\infty|^{1/2}](A+i)^{-1}$ in Hilbert–Schmidt norm.

Prove that $(A + B_n + i)^{-1} \to (A + B_\infty + i)^{-1}$ in trace norm.

51. The Klein–Gordon equation restricted to positive frequencies is a Schrödinger type equation $i\psi_t = H\psi$ with $H = \sqrt{-\Delta + V(x) + m_0^2}$ where V is such that $-\Delta + V \geq -m_0^2$. Let $H_0 = \sqrt{-\Delta + m_0^2}$. Prove that:

(a) If $V \in L^{3/2} + L^\infty$ and H is the square root of the operator defined as a form sum, then $C_0^\infty(\mathbb{R}^3)$ is an operator core for H.
(b) If $V \in L^1 \cap L^{3/2}$, then the wave operators $\Omega^\pm = \text{s-lim}_{t \to \mp\infty} e^{itH}e^{-itH_0}$ exist and are complete. (*Hint:* Use the invariance principle.)

†52. (a) Verify the form of H_0 under change to atomic coordinates by using the chain rule.
(b) Do the same for Jacobi coordinates.

53. In Lagrangian mechanics one defines momenta $p_1, \ldots, p_n$ conjugate to $q_1, \ldots, q_n$ by $p_i = \partial T/\partial \dot{q}_i$. Show that the formulas in Problem 52 can be derived by writing T in terms of the new conjugate momenta and letting p_i be $i^{-1}\,\partial/\partial q_i$.

†54. Fill in the details of the proof of part (a) of Theorem XI.38.

†55. Prove that

$$\lim_{\min|\mathbf{a}_i - \mathbf{a}_j| \to \infty} \int_0^\infty \|(I_{D'} - I_{D \cdot D'})e^{+i\tilde{H}_{D \cdot D'}t}U_D(\mathbf{a})e^{-iH_{D'}t}\psi\|\,dt = 0$$

if $\psi \in D(\tilde{H}_0)$, and thereby complete the proof of (77b).

†56. Use Theorem XI.39 to prove Theorem XI.40.

*57. Suppose that $V \in L^p \cap L^{3/2}(\mathbb{R}^3)$ with $1 < p < \frac{3}{2}$. By mimicking our proof of Theorem XI.41, prove an analogous theorem for $H = H_0 + V$.

58. Construct a function f, analytic in $\{z \mid \text{Im } z > 0\}$, continuous in $\{z \mid \text{Im } z \geq 0\}$ so that $z = 0$ is a limit point of zeros of f. (*Hint:* $\cos z$ has $z = \infty$ as a limit point of zeros.)

59. Using the Schwarz reflection principle, show that if f is analytic in $\{z \mid \text{Im } z > 0\}$, continuous in $\{z \mid \text{Im } z \geq 0\}$, then $\mathscr{E} = \mathbb{R} \cap \{z \mid f(z) = 0\}$ has an empty interior as a subset of $\mathbb{R}$.

†60. Let $V \in R$ and for $k \in \mathbb{R}$ let K_k be the operator on $L^2(\mathbb{R}^3)$ with kernel $K_k(x, y) = e^{ik|x-y|}(4\pi|x-y|)^{-1}|V(x)|^{1/2}V^{1/2}(y)$.

(a) Prove that $\text{Tr}(K_k^* K_k)$ is a constant.
(b) Using the Riemann–Lebesgue lemma, prove that $\text{Tr}(K_k^* K_k K_k^* K_k) \to 0$ as $k \to \infty$.
(c) Conclude that $\|K_k\| \to 0$ as $k \to \infty$.

Remark: This is a theorem of Klein and Zemach (see the notes to Section 6).

†*61*. (a) Let $V \in R \cap L^1(\mathbb{R}^3)$ and let $H_0 = -\Delta$; $H = H_0 + V$ (form sum). Prove that

$$(H - E)^{-1} = (H_0 - E)^{-1}$$
$$- [(H_0 - E)^{-1}V^{1/2}][1 + |V|^{1/2}(H_0 - E)^{-1}V^{1/2}]^{-1}[|V|^{1/2}(H_0 - E)^{-1}]$$

for $E \notin \sigma(H)$. (*Hint:* See Problem 46.)

(b) Using the integral equation

$$G(x, y; E) = G_0(x, y; E) - \int G_0(x, z; E)V(z)G(z, y; E)\, dz$$

prove that $G(\cdot, y; E) \in L^1$ for almost all y. (*Hint:* Use (a) to prove that $V^{1/2}G \in L^2$ a.e. in y.)

†*62*. Let $V \in R$ and let $H = H_0 + V$ (form sum). Suppose that $H\psi = E\psi$ for $E = k^2 \geq 0$ and ψ in $L^2(\mathbb{R}^3)$. Let $\varphi = |V|^{1/2}\psi$. Prove that

$$\varphi(x) = -\int |V(x)|^{1/2} \frac{e^{ik|x-y|}}{4\pi|x-y|} V(y)^{1/2}\varphi(y)\, dy$$

Conclude that $E \in \mathscr{E}$, the exceptional set.

†*63*. Fill in the details in the proof of Lemma 5 used in the proof of Theorem XI.41.

**64*. Suppose that $V(x) \leq 0$ for all x and $V \in L^1 \cap R$. Suppose that $-\Delta + V$ has a negative eigenvalue. Prove that the Born series for $T(0, 0)$ is not convergent.

65. The purpose of this problem is to prove (98).

(a) By using the scaling relation

$$G_0(x, y; E) = \lambda^{2-n}G_0(\lambda x, \lambda y; \lambda^2 E)$$

for $\lambda > 0$, show that it suffices to consider the case $|\text{Re } E| > 0$, $|E| = 1$.

(b) Write $G_0 = G_1 + G_2$ where

$$G_1 = (2\pi)^{-n} \int_{|p| \leq (1+\varepsilon)^2} (p^2 - E)^{-1} e^{ip\cdot(x-y)}\, d^n p$$

for some $\varepsilon > 0$. Prove that G_2 is analytic in the region $|E| < 1 + \varepsilon$ for each fixed $x \neq y$ and that $|G_2(x, y; E)| \leq |x - y|^{-(n-2)}$; $n \geq 3$.

(c) By shifting the contour of integration for $|p|$ in G_1, complete the proof of (98).

(d) Prove the $n = 1, 2$ analogues of (98) as described in the text.

(e) Prove the $\partial_i(-\Delta - k^2)^{-1}$ results by finding and proving an analogue of (98).

66. Let $H = -\alpha \nabla \cdot \beta \nabla \alpha = -f\Delta + g \cdot \nabla + h = -f_0 \Delta + V$ as in Theorem XI.45. Let $H_0 = -f_0 \Delta$ and $W = g \cdot \nabla + h$.

(a) Prove that $\|W\varphi\| \leq \varepsilon\|H_0\varphi\| + c_\varepsilon\|\varphi\|$ for any $\varepsilon > 0$ and that $\|W\varphi\| \leq \varepsilon\|-f\Delta\varphi\| + c_\varepsilon\|\varphi\|$.

(b) Prove that $\|-f\Delta\varphi\| \leq (1 + \varepsilon)\|H\varphi\| + c'_\varepsilon\|\varphi\|$.

(c) Prove that $\|(H - H_0)\varphi\| \leq a(\|H\varphi\| + \|H_0\varphi\|) + c\|\varphi\|$ for some $a < 1$.

(d) Conclude that H is self-adjoint on $D(H_0)$ by using Theorem X.13.

**67*. Use the method described at the end of the appendix to Section 6 to prove an eigenfunction expansion for $-\Delta + V$ on $L^2(\mathbb{R}^3)$ if V falls off exponentially.

*68. (a) Let $\langle M, \mu \rangle$ be a measure space and suppose that $K(x, y)$ and $F(x)K(x, y)F(y)^{-1}$ are in $L^2(M \times M, d\mu \otimes d\mu)$ for some F which is finite and nonzero almost everywhere. Let ψ be an L^2 solution of $\psi(x) = \int K(x, y)\psi(y)\, dy$. Prove that $F\psi \in L^2(M, d\mu)$.

†(b) Let M_k be the kernel given by (102c) and let K_k be the kernel of $|V|^{1/2}(H_0 - k^2)^{-1}V^{1/2}$. Prove that $(1 - M_k)$ is invertible if and only if $(1 - K_k)$ is invertible.

†69. Let V be a Rollnik potential, let $E < 0$, and let $H = H_0 + V$ as a form sum. Prove that $(H_0 + V)\psi = E\psi$ for some nonzero $\psi \in D(H)$ if and only if

$$(|V|^{1/2}(H_0 - E)^{-1}V^{1/2})\varphi = -\varphi$$

for some nonzero $\varphi \in L^2$ and that ψ and φ are related by $\varphi = |V|^{1/2}\psi$.

Reference for Problems 68, 69: Simon's monograph (see the notes to Section 6), pp. 149–150, 81–83.

†70. (a) Suppose that $e^{\alpha|x|}V(x) \in R$ for some $\alpha > 0$. Prove that $e^{\beta|x|}V(x) \in L^1(\mathbb{R}^3)$ for any $\beta < \alpha$.

(b) Suppose that $V \in R + L^\infty$ has compact support. Prove that V is in R.

†71. Prove that the poles of $(1 - M_k)^{-1}$ where M_k is given by (102c) are simple poles.

†72. Fill in the details in the proof of the corollary to Theorem XI.46.

†73. Use Theorem XI.42 to verify equation (105).

74. Let H be an N-body Hamiltonian so that every cluster Hamiltonian has no nondiscrete eigenvalues. Let $E = \inf \sigma(H)$. Verify that $[E, \infty) = \bigcup_{n=1}^{\infty} I_n$ where the I_n are disjoint intervals so that $\mathscr{C}_E$, the family of open channels at energy E, is constant on each I_n.

†75. Verify the properties (1)–(3) and (1′)–(3′) of $F_V(E)$ used in the proof of Theorem XI.49.

†76. Prove that the map $\langle V, E \rangle \mapsto K_V(E)$ from $R \times \mathbb{R}_+ \to \mathscr{I}_2$ (with R the Rollnik class) is jointly continuous.

†77. Prove part (c) of Theorem XI.49, that is, that when V is Rollnik, the T operator $T(E)$ goes to zero in norm as $E \to \infty$. (*Hint:* Consult the discussion of convergence of the Born series at high energy in Section 6 and see Problem 60.)

†78. Use the dominated convergence theorem to verify (118) when $V \in C_0^\infty$.

†79. (a) Verify the uniqueness of solutions of the variable phase equation (120) away from $r = 0$ by using uniqueness results from Section V.6.

(b) Prove that local solutions of the variable phase equation (120) extend to all of $(0, \infty)$ by verifying that d cannot go to infinity at any finite point.

(c) Use the variable phase equation to prove that any solution obeying $\lim_{r\to 0} |r^{-1}d(r)| < \infty$ actually obeys $\lim_{r\to 0} r^{-1}d(r) = 0$.

(d) Prove the existence and uniqueness of solutions near $r = 0$ by setting up a suitable contraction map.

80. Indicate the k-dependence in the variable phase equation by writing $d(r, k)$.

(a) Prove that $d(r, k)$ is continuous in k for each fixed r. (*Hint:* Use the existence proof.)

(b) Prove that $d(r, k) \to d_\infty(k)$ as $r \to \infty$ locally uniformly in k so that $d_\infty(k)$ is continuous. (*Hint:* Use the variable phase equation and the bound $\int_1^\infty |V(x)|\, dx < \infty$.)

(c) Prove that $d_\infty(k) \to 0$ as $k \to \infty$. (*Hint:* Prove it first for sufficiently small r and then use the variable phase equation and $\int_1^\infty |V(x)|\, dx < \infty$.)
(d) Conclude that $d_\infty(k) = \delta_0(k)$ without any π ambiguity.

†81. Derive (123) from (122).

82. Prove Corollary 2 to Theorem XI.54. (*Hint:* Use the methods of Problem 80.)

†83. In the context of Theorem XI.55, prove that if $\lim_{r\to\infty} u'(r) \neq 0$, then

$$\lim_{k\to 0} \frac{\delta_0(k^2) - m\pi}{k} = \lim_{r\to\infty} \frac{u(r) - ru'(r)}{u'(r)}$$

†84. (a) Prove the uniqueness statement of Theorem XI.56.
(b) Under the stronger hypothesis that $\int_0^1 |V(x)|\, dx < \infty$, prove the stronger uniqueness statement that the regular equation has a unique solution which remains bounded as $x \to 0$.

†85. (a) Prove that $|\sin u| \le [2|u|/(1 + |u|)]e^{|\mathrm{Im}\, u|}$ for all $u \in \mathbb{C}$.
(b) By writing

$$\frac{\sin k(x-y)}{k} = \frac{(\sin kx)e^{-iky} - e^{-ikx}\sin ky}{k}$$

prove that

$$\left|\frac{\sin k(x-y)}{k}\right| \le \frac{4y}{1 + |k|y} \exp[|\mathrm{Im}\, k|y + (\mathrm{Im}\, k)x]$$

for $0 \le x \le y$.
(c) Using the estimates in (a) and (b) fill in the details in the proof of Theorem XI.57.

†86. Prove Levinson's theorem in case $\eta(0) = 0$ by using Jost function methods. (*Hint:* Prove the simplicity of the zero at $k = 0$.)

87. Let S be a Borel set in $\mathbb{R}$. Let $A(S)$ be multiplication by x on $L^2(S, dx)$. Prove that:
(a) $A(S)$ is unitarily equivalent to $A(T)$ if and only if $S \,\Delta\, T$ has Lebesgue measure zero.
(b) The spectrum of $A(S)$ is $\bar{S}$.
(c) If there exists an isometry U with $A(S)U = UA(T)$, then $T\backslash S$ has Lebesgue measure zero.
(d) Under the hypothesis of (c), suppose also that T is closed and $\sigma(A(S)) = \sigma(A(T))$. Then U is unitary.
(e) If A is any operator with simple and purely absolutely continuous spectrum, then A is unitarily equivalent to some $A(S)$. S is called the **essential support of** A.

88. Let H and H_0 be two operators with simple spectrum. Suppose that $\sigma_{\mathrm{ac}}(H) \subset \sigma_{\mathrm{ac}}(H_0)$, that the essential support (see Problem 87) of the absolutely continuous part of H_0 is closed and that $\Omega^\pm(H, H_0)$ exist. Prove that $\Omega^\pm(H, H_0)$ are complete. Does the result still hold if the hypothesis on the essential support is removed?

†89. (a) Prove that a locally uniform limit of harmonic functions is harmonic. (*Hint:* Prove convergence as distributions and use elliptic regularity, or use Poisson's formula.)
(b) Prove that local L^1 convergence of harmonic functions implies local uniform convergence. (*Hint:* Use the mean-value property.)

†90. (a) If $z = \cos\theta$ with $\theta = x + iy$, prove that $|y| = a$ is the ellipse with foci ± 1 and semimajor axis $\cosh a$ by using the formula $\cos\theta = (\cos x)(\cosh y) + i(\sin x) \times (\sinh y)$.

(b) If $z \in \mathbb{C}\backslash(-1, 1)$ and x is small, prove that $\sum_{\ell=0}^{\infty} x^\ell Q_\ell(z) = g(x, z)$ where

$$g(x, z) = \frac{1}{u}\ln\left[\frac{z - x + u}{(z^2 - 1)^{1/2}}\right] = \frac{1}{2u}\ln\left[\frac{1 - (x - u)^2}{1 - (x + u)^2}\right]$$

and $u = (1 - 2zx + x^2)^{1/2}$.

(c) Prove that $g(x, z)$ has radius of convergence in x given by $e^{+|\operatorname{Im}\theta|}$ where $\theta = \cos^{-1}(z)$.

(d) Let D be a compact set outside the canonical ellipse $|\operatorname{Im}\theta| = \ln H$. Show that $\sup_{\ell;\, z \in D} |Q_\ell(z)H^\ell| < \infty$.

91. Prove (c) of Theorem XI.63. (*Hint*: Prove that $\lim_{\ell\to\infty} |P_\ell(z)|^{1/\ell} = e^{-|\operatorname{Im}\theta|}$ where $\theta = \cos^{-1}(z)$.)

*92. (a) Let $A = -d^2/dx^2$ on $L^2(-\infty, \infty)$. Let B_1 (respectively, B_2) be $-d^2/dx^2$ on $L^2(0, \infty)$ (respectively, $L^2(-\infty, 0)$) with zero boundary conditions at zero, and let $B = B_1 \oplus B_2$. Find explicit formulas for $(A + 1)^{-1}$ and $(B + 1)^{-1}$ and conclude that $0 \le (B + 1)^{-1} \le (A + 1)^{-1}$ (operator inequality).

(b) Prove that $(B + 1)^{-1/2}(A + 1)^{1/2}$ is bounded and conclude that $\partial(B_1 + 1)^{-1/2}$ is bounded (where $\partial f = \partial f/\partial r$) and that $W(B_1 + 1)^{-1/2}$ is trace class if $W \in L^2_\delta(\mathbb{R})$ for $\delta > \frac{1}{2}$ (See Theorem XI.21.)

(c) Let $V = \partial W - W\partial =$ multiplication by $\partial W/\partial r$. Under the hypothesis that $W \in L^2_\delta(\mathbb{R})$, prove that V is a form-bounded perturbation of B_1 with relative bound zero and that $(B_1 + V + i)^{-1} - (B_1 + i)^{-1}$ is trace class.

(d) Let W be a function of $|x|$ on $\mathbb{R}^n$ with $\int |W(r)|^2(1 + r^2)^{-\frac{1}{2}-\varepsilon}\, dr < \infty$ for some $\varepsilon > 0$. Let $V = \partial W/\partial r$. Prove that $\Omega^\pm(-\Delta + V, -\Delta)$ exist and are complete.

†93. (a) Prove the bound $|u_n'(x)| \le n\gamma^n \|u_0\| A(x)$ needed in the proof of the proposition in Appendix 2 to Section 8.

(b) Extend the proof of the proposition to the case where $u_0(x)$ is x-dependent.

94. Let u obey (151). Prove that for all $f \in L^2(0, \infty)$ which have compact support in $(0, \infty)\backslash\mathscr{E}$, $\int f(k)u(k, r)\, dk \in L^2(0, \infty)$. (*Hint*: Write the integral in the two pieces suggested by (151). Control the $(1 + |r|)^{-\frac{1}{2}-\gamma}$ term by using $f \in L^1$ and the other term by the Plancherel theorem.)

*95. (a) Suppose that u obeys (151) and in addition that

$$\left|\frac{\partial u}{\partial r}(r, k) - k\cos\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)\right| \le c(k)(1 + |r|)^{-\frac{1}{2}-\gamma} \tag{356}$$

Prove that if f is as in Problem 94, then $Y_{\ell m}(\hat{x}) \int (kx)^{-1} f(k)u(kx)\, dk$ is in the form domain of $-\Delta$.

(b) If (356) holds, show that "$-\Delta + V$ essentially self-adjoint on C_0^∞" can be replaced by "C_0^∞ is a form core for $H = -\Delta + V$ and $Q(H) = Q(-\Delta)$" in the hypotheses of Theorem XI.69.

(c) Apply the extension given in (b) to the potential $(1 + |r|^2)^{-1}e^r\cos(e^r)$.

†96. Provide the details of the proof of Theorem XI.70.

97. (a) Let $A(y)$ and $T(y)$ be matrix-valued functions so that $T(y)$ is invertible, $\|T(x)T(y)^{-1}\| \leq 1$, if $x \leq y$, and so that $\tilde{A}(y) = T(y)A(y)T(y)^{-1}$ obeys $\int_R^\infty \|\tilde{A}(y)\|\,dy < 1$. Suppose that $T(y)u_0 = u_0$ for all y. Show that $u(x) = u_0 + \int_x^\infty A(y)u(y)\,dy$ has a solution. (*Hint:* Estimate $T(x)u_n(x)$ inductively.)

(b) Let $f(x)$ be a positive monotone increasing function and $\tilde{A}$ a 2×2 matrix in L^1. Show that

$$\dot{u}(t) = -\begin{pmatrix} \tilde{a}_{11}(t) & \tilde{a}_{12}(t)f(t) \\ \tilde{a}_{21}(t)f(t)^{-1} & \tilde{a}_{22}(t) \end{pmatrix} u(t)$$

has a solution approaching $\langle 1, 0 \rangle$ at infinity.

(c) Construct a solution of

$$-u''(x) + x^{2n}u(x) = 0$$

which is asymptotic to $\exp(-(n+1)^{-1}x^{n+1})$ as $x \to \infty$. (*Hint:* Use variation of parameters with the two solutions $\exp(\pm(n+1)^{-1}x^{n+1})$.)

(d) Suppose that $A = A_1 + A_2$ where $\tilde{A}_1(y) = T(y)A_1(y)T(y)^{-1}$ is in L^1 and that $A_2(y) = dB(y)/dy$ with $\tilde{B}(y) = T(y)B(y)T(y)^{-1}$ obeying $\tilde{A}\tilde{B} \in L^1$ and $\tilde{B} \to 0$ at infinity. Suppose that $T(y)u_0 = u_0$. Show that $\dot{u}(t) = A(t)u(t)$ has a solution satisfying $u(t) \to u_0$ at infinity.

(e) Let $f(x)$ be a positive monotone increasing function so that $|\dot{f}(t)| \leq ct^{-\alpha}|f(t)|$. $t \geq R$, $\alpha > 0$. Let $\tilde{A}(t)$ be a 2×2 matrix-valued function with $\tilde{A} = M_1 + \dot{M}_2$ where $M_1 \in L^1$, $\tilde{A}M_2 \in L^1$, $t^{-\alpha}M_2 \in L^1$, and $M_2 \to 0$ at infinity. Show that

$$\dot{u}(t) = \begin{pmatrix} \tilde{a}_{11}(t) & \tilde{a}_{12}(t)f(t) \\ \tilde{a}_{21}(t)f(t)^{-1} & \tilde{a}_{22}(t) \end{pmatrix} u(t)$$

has a solution converging to $\langle 1, 0 \rangle$ at infinity.

98. (a) Let f and g be functions in $C^1(\mathbf{R})$ so that $fg' - gf'$ is everywhere nonvanishing. Suppose that $\langle u(x), u'(x) \rangle$ and $\langle a(x), b(x) \rangle$ are related by the formulas:

$$u(x) = a(x)f(x) + b(x)g(x)$$
$$u'(x) = a(x)f'(x) + b(x)g'(x)$$

Let $W(x)$ be given. Prove that the differential equation $u''(x) = W(x)u(x)$ is equivalent to the differential equation $\rho'(x) = \Delta(x)\rho(x)$ where $\rho(x) = \langle a(x), b(x) \rangle$ and

$$\Delta = (f'g - gf')^{-1} \begin{pmatrix} -g(-f'' + Wf) & -g(-g'' + Wg) \\ f(-f'' + Wf) & f(-g'' + Wg) \end{pmatrix}$$

(b) Prove Theorem XI.67c by using Problem 97e and part (a) with the choice

$$f(x) = x^{-\gamma_j/2\alpha_j} \cos(\alpha_j x/2)$$
$$g(x) = x^{\gamma_j/2\alpha_j} \sin(\alpha_j x/2)$$

99. Prove (155) and conclude that the ordinary wave operators do not exist in the Coulomb case. (*Hint:* First prove that $(1 - P_{\text{ac}}(H))e^{itH}e^{-itH_0} \to 0$ weakly. Then, using the fact that $U_D(t)^* e^{-itH} P_{\text{ac}}(H)$ converges, prove that $P_{\text{ac}}(H)e^{itH}e^{-itH_0} \to 0$ weakly.)

†*100.* Let $W(k, t)$, $P(k)$ be real-valued functions so that for each s and almost every k,

$$W(k, t + s) - W(k, t) \to sP(k)$$

as $t \to \pm\infty$. Prove that

$$\operatorname*{s-lim}_{t \to \pm\infty} \exp(iW(i\nabla, t)) \exp(-iW(i\nabla, t + s)) = \exp(-isP(i\nabla))$$

(*Hint*. Use dominated convergence.)

†*101.* Use the method of stationary phase to prove (159a).

102. Let $H_0 = -\Delta$; $H = -\Delta - \lambda r^{-1} + V_s$; $H' = -\Delta - \lambda r^{-1}$. Let $\varphi \in C_0^\infty$ with $\varphi \equiv 1$ near $r = 0$. Let $\tilde{H} = H_0 - \lambda(1 - \varphi)r^{-1}$; $W = -\lambda r^{-1}\varphi$.

(a) Prove that $\Omega_D^\pm(H, H_0) = \Omega^\pm(H, H')\Omega_D^\pm(H', H_0)$ and conclude that to prove completeness of $\Omega_D^\pm(H, H_0)$ it suffices to prove completeness of $\Omega_D^\pm(H', H_0)$ and $\Omega^\pm(H, H')$.

(b) Suppose that $V_s(H_0 + 1)^{-m-1}$ is trace class. Prove that $V_s(\tilde{H} + E)^{-m-1}$ is trace class by proving that $D(H_0^{m+1}) = D(\tilde{H}^{m+1})$.

(c) Prove that $W(H_0 + 1)^{-m-1}$ is trace class for m large enough.

(d) Prove that $(\tilde{H} + E)^{-m} - (H' + E)^{-m}$ and $(\tilde{H} + E)^{-m} - (H + E)^{-m}$ are trace class if $V_s(\tilde{H} + E)^{-m-1}$ is trace class so long as m is sufficiently large.

(e) Prove that if $V_s(H_0 + 1)^{-m-1}$ is trace class, then $\Omega^\pm(H, H')$ exist and are complete.

Remark: $\Omega_D^\pm(H', H_0)$ are complete by an explicit eigenfunction expansion; see Dollard's basic paper quoted in the notes to Section 9.

103. Verify that in the long-range classical case $(\Sigma_+ \backslash \Sigma_-) \cup (\Sigma_- \backslash \Sigma_+)$ has measure zero and that (167) holds for every $\langle x_0, p_0 \rangle$ in $\Sigma_\pm$.

104. Use a contraction mapping argument of the type used in Section 2 to prove the existence of solutions of (172).

105. Prove that for almost all p_{in}, b_{in}, the corresponding long range solution $x(t)$ associated with (172) obeys $\lim_{t \to \infty} |x(t)| = \infty$. (*Hint*: Let G be the map of $\langle p_{\text{in}}, a \rangle$ into the solution associated with (172) at time $t = 0$. Prove that G is measure preserving.)

106. Fix $\alpha > 0$. Suppose that $\sup_x [(1 + x)^{\alpha + |\beta|} |D^\beta(V_n - V)|] \to 0$ for $|\beta| \le 2$. Let $N = [1/\alpha]$.

(a) Prove that the function $z_N(p, t; V_n)$ converges uniformly in t for p in compact subsets of $\mathbb{R}^n \backslash \{0\}$ to $z_N(p, t; V)$.

(b) Prove that the solutions of (172) associated with V_n converge as $n \to \infty$ to that for V.

(c) Prove that the map $\tilde{S}$ of Theorem XI.73 converges as $n \to \infty$.

(d) Prove that if V_n is short-range, the $\tilde{S}$ defined with z_N is identical to part of the usual short-range S.

**107.* Using Hörmander's results on solutions of the Hamilton–Jacobi equation, improve Herbst's analysis of classical long-range scattering via canonical transformations. *References*: The Hörmander paper and the second Herbst paper quoted in the notes to Section 9.

108. (a) Let $W(k, t)$ be a real-valued function so that for some fixed H, $e^{iHt} \exp(-iW(-i\nabla, t)) \to \Omega_D^+$ as $t \to -\infty$. Let P_D be the projection on $\operatorname{Ran} \Omega_D^+$.

Prove that for any other measurable function $\tilde{W}(k, t)$, there is an L^∞ function $G(k)$ and a subnet $t_\alpha \to -\infty$, so that

$$\underset{t_\alpha \to -\infty}{\text{w-lim}}\, P_D e^{iHt} \exp(-i\tilde{W}(-i\nabla, t_\alpha)) = \Omega_D^+ G(-i\nabla)$$

(*Hint:* Let $G(k)$ be a limit point of $\exp(iW(k, t) - i\tilde{W}(k, t))$ in the $\sigma(L^\infty, L^1) = w^*$-topology.)

(b) If $\text{s-lim}_{t \to -\infty}\, e^{iHt} \exp(-i\tilde{W}(-i\nabla, t)) = \tilde{\Omega}_D^+$ exists, prove that $P_D \tilde{\Omega}_D^+ = \Omega_D^+ G(-i\nabla)$.
(c) If, moreover, $P_D = P_{ac}(H)$, prove that $|G(k)| = 1$ a.e.

109. Let V obey $|D^\alpha V(x)| \le C(1 + x)^{-|\alpha| - \varepsilon}$ for all α with $|\alpha| \le 3$. Prove that one can write $V = V_1 + V_2$ where $|V_2(x)| \le C(1 + x)^{-1-\varepsilon}$ and $|(D^\alpha V_1)(x)| \le C(1 + x)^{-m(|\alpha|)}$ where $m(\ell) = +\ell + \varepsilon$ for $\ell = 0, 1, 2, 3$ and $m(\ell) = 3 + \varepsilon + \frac{2}{3}(\ell - 3)$ for $\ell \ge 3$, by the following steps:

(a) Pick $\psi \in C_0^\infty(\mathbb{R}^n)$ with $\psi(x) = 1$ if $|x| \le 1$, $\psi(x) = 0$ if $|x| \ge 2$, and $0 \le \psi(x) \le 1$ for all x. Let $\psi_\nu(x) = \psi(2^{-\nu}x) - \psi(2^{1-\nu}x)$ and $V_\nu = V\psi_\nu$. Prove that $\|D^\alpha \psi_\nu\|_\infty \le C_\alpha 2^{-\nu|\alpha|}$, that $|(D^\alpha \psi_\nu)(x)| \le d(1 + |x|)^{-|\alpha|}$ and conclude that $|D^\alpha V_\nu(x)| \le C(1 + x)^{-|\alpha| - \varepsilon}$, $0 \le \alpha \le 3$.
(b) Let $\delta = \frac{2}{3}$. Let $\chi \in C_0^\infty(\mathbb{R}^n)$ with $\int \chi(x)\, dx = 1$ and $\int |x|^\alpha \chi(x)\, dx = 0$ for $0 < |\alpha| < 3$. Let $\chi_\nu(y) = 2^{-\delta n \nu}\chi(2^{-\nu\delta}y)$. Prove that

$$\left| V_\nu(x - y) - V_\nu(x) - \sum_{1 \le |\alpha| \le 2} (\alpha!)^{-1}(y)^\alpha (D^\alpha V_\nu)(x) \right| \le C|y|^3(1 + x)^{-3-\varepsilon}$$

for all x, y with $x \in \operatorname{supp} V_\nu$ and $y \in \operatorname{supp} \chi_\nu$. Conclude that

$$|\chi_\nu * V_\nu(x) - V_\nu(x)| \le C(1 + x)^{-1-\varepsilon}$$

(c) Prove that $D^\alpha(V_\nu * \chi_\nu) \le C_\alpha(1 + x)^{-m(|\alpha|)}$.
(d) Complete the proof by taking $V_1 = \sum_\nu V_\nu * \chi_\nu$ and $V_2 = V - V_1$.

110. By following the method of Problem 109, show that if $|D^\alpha V(x)| \le C(1 + x)^{-|\alpha| - \varepsilon}$, $|\alpha| \le M$ where $\varepsilon > \frac{1}{2}$ for $M = 1$ and $\varepsilon > \frac{1}{5}$ for $M = 2$, then $V = V_1 + V_2$ where $|V_2(x)| \le C(1 + x)^{-1-\varepsilon}$ and $|(D^\alpha V_1)(x)| \le C(1 + x)^{-m(|\alpha|)}$ where $m(1) + m(3) > 4$.

Reference for Problems 109 and 110: Hörmander's paper quoted in the notes to Section 9.

111. (a) Compute the classical Coulomb differential cross section (Rutherford cross section).
(b) Compute the Coulomb cross section in the Born approximation.

†*112.* Using the notation of Theorem XI.75 in Section 10, show that
(a) $\langle u, v\rangle \in P_{ac}(A_0) \Leftrightarrow B_0 u \in P_{ac}(B_0)$ and $v \in P_{ac}(B_0)$.

(b) $T_0 P_{ac}(A_0) = \begin{pmatrix} P_{ac}(B_0) & 0 \\ 0 & P_{ac}(B_0) \end{pmatrix}$.

†*113.* Assuming that Theorems XI.75 and XI.76 continue to hold if H_0 and H_1 have point spectrum at zero, fill in the details of the proof of the existence of the wave operators for optical scattering in inhomogeneous media (Example 2 of Section 10).

114. Using the methods of Section 10, develop a scattering theory for the wave equations

$$u_{tt} - \Delta u = 0$$

$$u_{tt} - \Delta u + q(x)u = 0$$

under appropriate conditions on $q(x)$.

115. Let A and B be bounded operators on a Hilbert space $\mathscr{H}$.
(a) Prove that $\sigma(AB)\backslash\{0\} = \sigma(BA)\backslash\{0\}$.
(b) Prove the commutation formula (205).

**116.* The purpose of this problem is to extend Theorems XI.79 and XI.80 to $n \neq 3$ dimensions.
(a) Use the method of proof of Theorem XI.21 to prove that $(1 + x^2)^{-\alpha}(1 + p^2)^{-\beta} \times (1 + x^2)^{-\gamma} \in \mathscr{I}_p$ as operators on $L^2(\mathbf{R}^n)$ so long as $\beta > n/2p$, $\alpha + \gamma > n/2p$ where α or γ may be negative. (*Hint:* Consider first the case $p \geq 2$ and then write

$$\begin{aligned}(1 + x^2)^{-\alpha}&(1 + p^2)^{-\beta}(1 + x^2)^{-\gamma}\\ &= [(1 + x^2)^{-\alpha}(1 + p^2)^{-\beta/2}(1 + x^2)^{-\delta}][(1 + x^2)^{\delta}(1 + p^2)^{-\beta/2}(1 + x^2)^{-\gamma}]\end{aligned}$$

for suitable δ.)
(b) Let $R_0 = (H_0 + 1)^{-1}$ and let R be another operator. Suppose that $(1 + x^2)^k \times (R - R_0)(1 + x^2)^k \in \mathscr{I}_p$ for $p > \frac{1}{2}n$ and all k. Prove inductively that $(1 + x^2)^k \times (R^m - R_0^m)(1 + x^2)^k \in \mathscr{I}_p$ for all k, all $m = 1, 2, 3, \ldots$ and $p > n/2m$ and in particular that $R^m - R_0^m \in \mathscr{I}_1$ if $m > n/2$.
(c) Prove suitable analogs of Theorems XI.79 and XI.80 for any n.

117. We say that positive self-adjoint operators A and B obey $A \leq B$ if and only if $Q(B) \subset Q(A)$ and $(\varphi, A\varphi) \leq (\varphi, B\varphi)$ for all $\varphi \in Q(B)$. Suppose that A and B have bounded inverses. Prove that $B^{-1} \leq A^{-1}$. *Hint:*

$$\begin{aligned}(\varphi, B^{-1}\varphi) &\leq (A^{-1}\varphi, AB^{-1}\varphi)\\ &\leq (A^{-1}\varphi, \varphi)^{1/2}(B^{-1}\varphi, AB^{-1}\varphi)^{1/2}\\ &\leq (\varphi, A^{-1}\varphi)^{1/2}(\varphi, B^{-1}\varphi)^{1/2}.\end{aligned}$$

†*118.* Fill in the details of the proof of Theorem XI.81′.

119. Let W be a bounded closed subset of $\mathbf{R}^2$ and let $\Gamma = \{\langle x_1, x_2, x_3\rangle \in \mathbf{R}^3 \,|\, \langle x_1, x_2\rangle \in W, x_3 = 0\}$. The purpose of this problem is to prove that $R_{\Gamma,\mathrm{N}}^2 - R_0^2$ is trace class.
(a) Show that Theorem XI.80 can be modified to allow the sphere S to be replaced by the boundary of a cube C.
(b) Let C be a cube and let Γ' be a piece of hyperplane slicing C into two rectangular parallelopipeds. Prove, that $\tilde{R}_{\partial C \cup \Gamma;\mathrm{N}}$, the Laplace operator on $L^2(C)$ with Neumann boundary conditions on $\partial C \cup \Gamma'$, is Hilbert–Schmidt. (*Hint:* Compute the eigenvalues of $\tilde{R}$!)
*(c) Complete the proof that $R_{\Gamma;\mathrm{N}}^2 - R_0^2$ is trace class.

120. In the case of Dirichlet obstacle scattering, we showed that $\Omega^{\pm}(A_{\mathrm{D}}, A_0; I_{10}^*)$ exist. Let J be multiplication (on both components) by a function $\varphi \in C_0^\infty$ vanishing in a neighborhood of the obstacle. Show that $\Omega^{\pm}(A_{\mathrm{D}}, A_0; J)$ exist.

121. Prove uniqueness of the representations in Theorem XI.82 and XI.83.

122. (a) Let $d\nu(\theta)$ be a translation invariant Borel measure on the circle. Prove that $d\nu = c\, d\theta$. (*Hint:* Apply Fubini's theorem to $\int f(\theta + \theta')\, d\nu(\theta)\, d\theta'$.)
(b) Let $d\nu(x)$ be a translation invariant Borel measure on $\mathbb{R}$. Prove that $d\nu(x) = c\, dx$.

†*123.* Prove that the operator valued function $t(\sigma + iy)$ is norm analytic in the upper half-plane by using the fact that it is weakly analytic and the ideas of Theorem VI.4.

**124.* Using the ideas in Example 3 of Section 11, verify the hypotheses of Theorem XI.91 for the interacting group of Example 2.

125. Under the additional hypothesis $q > 1$ in Theorem XI.98, prove that $\|e^{iAt}\varphi(t) - \varphi_+\|_{\text{scat}} \to 0$ as $t \to +\infty$.

†*126.* Prove that the scattering operator on small data constructed in Theorem XI.98 is one to one. (*Hint:* Turn around the uniqueness part of Theorem XI.97.)

127. (a) Let g be a positive integrable function on $\mathbb{R}$ and suppose that f is measurable, bounded on each interval $(-\infty, t)$, and satisfies

$$f(t) \le c_0 + b_0 \int_{-\infty}^{t} f(s) g(s)\, ds \qquad \text{for all } t$$

Prove that

$$f(t) \le c_0 \exp\left(b_0 \int_{-\infty}^{t} g(s)\, ds\right) \qquad \text{for all } t$$

*(b) Let α and β be two Hermitian two by two matrices that satisfy

$$\alpha^2 = I = \beta^2, \qquad \beta\alpha + \alpha\beta = 0$$

Prove global existence for the coupled Klein-Gordon and Dirac equations in one dimension:

$$\frac{\partial \psi}{\partial t} + i\left(i\alpha \frac{\partial}{\partial x} - m_e \beta\right)\psi = -ig\beta u\psi$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + m_0^2 u = \bar{\psi} \cdot \beta\psi$$

where g is a real coupling constant, $u(x, t)$ is a real-valued function on $\mathbb{R}^2$, $\psi(x, t)$ is a $\mathbb{C} \times \mathbb{C}$ valued function on $\mathbb{R}^2$, and $\bar{\psi} \cdot \beta\psi$ denotes the dot product. (*Hint:* Find conserved quantities, use the Sobolev estimate $\|f\|_\infty \le c\|f'\|_2^{1/2}\|f\|_2^{1/2}$, and iterate like mad.)

Reference: J. Chadam, "Global solutions of the Cauchy problem for the (classical) coupled Maxwell-Dirac equations in one space dimension," *J. Functional Anal.* **13** (1973), 173–184.

†*128.* Fill in the details of the proof of Theorem XI.100. In particular:
(a) Show that for each t and η, M_t is uniformly continuous on $\{\psi \in \Sigma_{\text{scat}} \mid \|\psi\|_{\text{scat}} \le \eta\}$ in the $\|\cdot\|_{\text{scat}}$ topology. (*Hint:* First show that M_t is continuous in the $\|\cdot\|$ topology.)
(b) Prove that Ω^+ is one-to-one.

129. (a) Let $B = \sqrt{-\Delta + m^2}$ on $L^2(\mathbb{R}^3)$. Show that there is a constant c so that

$$\|B^{-1}\sin[(t-s)B]u^3(s)\|_\infty \le C\|Bu(s)\|_2\,\|u(s)\|_\infty^2$$

for each $u(s) \in D(B^2) \subset L^2(\mathbb{R}^3)$.

(b) Use this estimate and the techniques of Theorem XI.100 to construct the wave operators for

$$u_{tt} - \Delta u + m^2 u = -u^3$$

in the case $n = 3$.

130. Prove global existence for the nonlinear Schrödinger equation (261) for $p \ge 1$ and $\lambda > 0$.

Note: Problems 131, 132, 133 require some familiarity with the quantum theory of addition of angular momentum.

131. Let $\boldsymbol{\sigma}^{(\alpha)}$ and $\boldsymbol{\sigma}^{(\beta)}$ be Pauli spins at different sites in a Heisenberg model. Let $k_{\alpha\beta}$ be defined by $k_{\alpha\beta} = (\boldsymbol{\sigma}^{(\alpha)} + \boldsymbol{\sigma}^{(\beta)})^2$. Prove that $k_{\alpha\beta}$ has the eigenvalues 0 and 8 and that $\boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)} = 1$ when $k_{\alpha\beta} = 8$ and $\boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)} = -3$ when $k_{\alpha\beta} = 0$.

**132.* (a) Let $\boldsymbol{\sigma}^{(\alpha)}, \boldsymbol{\sigma}^{(\beta)}, \boldsymbol{\sigma}^{(\gamma)}$ be three Pauli spins at different sites. Prove that

$$(1 - \boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)}) \le 2(1 - \boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\gamma)}) + 2(1 - \boldsymbol{\sigma}^{(\beta)} \cdot \boldsymbol{\sigma}^{(\gamma)})$$

as an operator inequality.

(b) Let $H = -\sum J_{\alpha\beta}\boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)}$ be a finite sum with each $J_{\alpha\beta} \ge 0$ so that the sites cannot be broken into two noninteracting groups. Prove that the lowest eigenvalue of H is $-\sum J_{\alpha\beta}$ and that this eigenvalue has multiplicity $n + 1$ where n is the number of sites. (*Hint:* Use (a) to prove that every eigenvector with eigenvalue $-\sum J_{\alpha\beta}$ has total angular momentum $S = \frac{1}{2}(\sum \sigma_\alpha)$ with $s = \frac{1}{2}n$.)

**133.* (a) Let $\boldsymbol{\sigma}^{(\alpha)}, \boldsymbol{\sigma}^{(\beta)}$ be Pauli spins at two different sites. Let ρ be a density matrix with $\operatorname{Tr}(\rho\boldsymbol{\sigma}^{(\alpha)} \cdot \boldsymbol{\sigma}^{(\beta)}) = 1$. Prove that $\operatorname{Tr}(\rho\boldsymbol{\sigma}^{(\alpha)}) = \operatorname{Tr}(\rho\boldsymbol{\sigma}^{(\beta)})$.

(b) Let $\psi \in \mathscr{H}_n$, the n spin space for the infinite volume system. Prove that

$$\lim_{\Lambda \to \infty}\left(\psi, \sum_{\alpha \in \Lambda} \tfrac{1}{2}(\sigma_z^{(\alpha)} + 1)\psi\right) = n$$

(c) Let H be the infinite volume Hamiltonian for the zero temperature Heisenberg model. Let $\psi \in \mathscr{H}_n$ with $H\psi = 0$. Prove that $(\psi, \sigma_z^{(\alpha)}\psi)$ is independent of α and conclude that $n = 0$.

†134. Verify (276).

**135.* Let $H_2(K)$ be the fibering described at the end of Section 14. Let $J_2(K)$ and $H_2^{(0)}(K)$ be the corresponding fibering for J_2 and $H_1^{\otimes}$. Prove that

$$H_2(K)J_2(K) - J_2(K)H_2^{(0)}(K)$$

is finite rank and thus trace class. Conclude that $\operatorname{Ran}\Omega_2^+ = \operatorname{Ran}\Omega_2^-$.

136. Show that the inner product (344) is well defined by showing that if v and w have different representations as finite linear combinations of vectors in D_0, then (v, w) is independent of the representation chosen.

†*137.* In the proof of Theorem XI.104, verify that the operators $h(t) + M + 1$ satisfy the hypotheses of Theorem X.70.

†*138.* Verify part (e) of Theorem XI.104.

†*139.* Check that the charged scalar field of mass m obeys the obvious extension of the Gårding–Wightman axioms.

†*140.* Generalize the causality proof in Section 15 to show that $[\varphi(f, t), \varphi(g, t')^*] = 0$ whenever $\{\langle x, t\rangle \mid x \in \operatorname{supp} f\}$ and $\{\langle x, t'\rangle \mid x \in \operatorname{supp} g\}$ are spacelike separated.

†*141.* Fill in the following details of the proof of Theorem XI.106:

(a) Complete the proof of (295).

(b) Prove that

$$(a_i + \lambda_i b_i^*)e^{-\lambda_i a_i^* b_i^*}\psi_{\text{in}} = 0$$

(c) Fill in the details of the proof that S^{-1} is an isometry.

142. Fix a short-range potential V in $\mathbb{R}^3$. Let $\mathcal{F}$ be the Boson Fock space built on $L^2(\mathbb{R}^3)$, that is, $\mathcal{F}_n = L_s^2(\mathbb{R}^{3n})$, the functions $f(x_1, \ldots, x_n)$ on $\mathbb{R}^{3n}$ which are symmetric. Define a Hamiltonian H on $\mathcal{F}$ by requiring that H leave $\mathcal{F}_n$ invariant, V be even, and that

$$H \restriction \mathcal{F}_n = -\sum_{i=1}^{n} \Delta_i + \sum_{i<j} V(x_i - x_j)$$

Let Ω_0 be the Fock vacuum and define a "field operator" by

$$\varphi(x, 0) = (2\pi)^{-3/2} \int [e^{-ip\cdot x}a^\dagger(p) + e^{+ip\cdot x}a(p)]\, d^3p/\sqrt{2}$$

$$\varphi(x, t) = e^{itH}\varphi(x, 0)e^{-itH}$$

By a regular wave packet for the free Schrödinger equation, we mean a function $f(x, t)$ of the form

$$f(x, t) = (2\pi)^{-3/2} \int e^{-ip^2t}e^{ip\cdot x}g(p)\, d^3p$$

with $g \in C_0^\infty(\mathbb{R}^3)$. Given such an f, define $\varphi_f(t)$ by

$$\varphi_f(t) = \int \varphi(x, t)f(x, t)\, d^3x$$

(a) Prove that for any regular wave packets $f_1, \ldots, f_n$,

$$\eta(t) \equiv \varphi_{f_1}(t) \cdots \varphi_{f_n}(t)\Omega_0$$

has a limit as $t \to \pm\infty$ in the norm topology by writing $\eta(t)$ as $e^{itH}e^{-itH_0}g$ for suitable g and using the known facts about nonrelativistic scattering.

(b) Prove (a) by mimicking the Haag–Ruelle method. (*Hint:* The TVEV at equal time are extremely simple; compute them exactly!)

(c) Suppose that $H \restriction \mathcal{F}_2$ has a bound state. Introduce suitable new "field" operators ψ so that the procedure in (a) will yield channel wave operators with this bound state if ψ fields are used and channel wave operators for free particles and this bound state if φ and ψ are used.

References: The Hepp lectures and Sandhas article quoted in the notes to Section 16.

143. Prove that the TVEV are given explicitly in terms of the Wightman distributions by

$$\mathscr{W}_{n,T}(x_1, \ldots, x_n) = \sum_{P \in \mathscr{P}_n} (-1)^{(|P|+1)} c_p \mathscr{W}_{k_1}(x_{i_1}, \ldots, x_{i_k}) \cdots \mathscr{W}_{k_\ell}(x_{i_1'}, \ldots, x_{i'_{k'}})$$

where $|P| = \ell$ and

$$c_p = \begin{cases} 1, & |P| = 1 \\ |P| - 1, & |P| \geq 2 \end{cases}$$

144. Suppose that for $n = 1, 2, \ldots$ we are given functions $f_n(\lambda)$ on $(0, \infty)$ with asymptotic series $f_n(\lambda) \sim \sum_m a_{n,m} \lambda^m$. Define "truncated" functions $f_{n,T}(\lambda)$ inductively by

$$f_n(\lambda) = \sum N(m_1, \ldots, m_k) f_{m_1,T}(\lambda) \cdots f_{m_k,T}(\lambda)$$

where $N(m_1, \ldots, m_k)$ is the number of distinct partitions of $\{1, \ldots, n\}$ into k sets with $m_1, \ldots, m_k$ elements (so $N = n!/m_1! \cdots m_k!$ if the m_i are distinct but it is less if some m_i are equal). By an n, m graph, we mean a set of n labeled red points and m labeled black points joined together by some set of lines. To each graph Γ we define a value $V(\Gamma)$ with two restrictions: (i) The value is independent of permutation of the labels of the red (respectively, black) points. (ii) The value of any graph Γ which is a "union" of connected graphs $\Gamma_1, \ldots, \Gamma_k$ is $V(\Gamma) = V(\Gamma_1) \cdots V(\Gamma_k)$. Suppose that

$$a_{n,m} = \sum_{\Gamma,\text{ an } n,\, m \text{ graph}} V(\Gamma).$$

Prove that $f_{n,T}(\lambda) \sim \sum a_{n,m}^{T} \lambda^m$ where

$$a_{n,m}^{T} = \sum_{\Gamma \text{ a connected } n,\, m \text{ graph}} V(\Gamma)$$

Remark: It is only for notational convenience that we did not let $f_n(\lambda)$ depend on n points $x_1, \ldots, x_n$ obtaining a family of Wightman distributions and TVEVs in this way. The analogue of this result in that case has the following consequence: In those theories where the $\mathscr{W}_n$ are given "formally" as sums of Feynman diagrams, the TVEV are given as sums of connected Feynman diagrams. It also means that the "connected" S-matrix of Section 5 is related to the full S-matrix as the TVEV are related to the VEV.

†*145.* Verify (314). (*Hint:* Prove that $\mathbf{a} \cdot \mathbf{P}$ has purely absolutely continuous spectrum on $\{\psi_0\}^\perp$ and use the Riemann–Lebesgue lemma.)

†*146.* (a) Show that the support property of the $\hat{W}_n$ (Theorem IX.32) is equivalent to saying that the support of the $\hat{\mathscr{W}}_n$ is

$$S_n = \{\langle q_1, \ldots, q_n\rangle \mid q_1 \in -\bar{V}_+, q_1 + q_2 \in -\bar{V}_+, \ldots, q_1 + \cdots + q_{n-1} \in -\bar{V}_+,$$
$$q_1 + \cdots + q_n = 0\}$$

(*Hint:* $\sum_{i=1}^{n} q_i x_i = \sum_{i=1}^{n-1} (x_i - x_{i+1})(\sum_{j=1}^{i} q_j) + x_n \sum_{j=1}^{n} q_j$.)

(b) Let $\langle i_1, \ldots, i_{k_1}\rangle, \ldots, \langle i_1', \ldots, i_{k_\ell}'\rangle$ be a partition of $\{1, \ldots, n\}$ with $i_1 < \cdots < i_{k_1}$; etc. Let

$$G(x_1, \ldots, x_n) = \mathscr{W}_{k_1}(x_{i_1}, \ldots, x_{i_{k(1)}}) \cdots \mathscr{W}_{k_\ell}(x_{i'_1}, \ldots, x_{i'_{k(\ell)}})$$

Prove that $\hat{G}$ has support in S_n.

(c) If $\hat{\mathscr{W}}_{n,T}$ is used in (a), show that $-\bar{V}_+$ can be replaced by $-\bar{V}_{+,m}$ if Property 9 is assumed.

(d) Let $\langle q_1, \ldots, q_n\rangle$ be in the support of $\hat{\mathscr{W}}_{n,T}(x_{i_1}, \ldots, x_{i_k}, x_{i'_1}, \ldots, x_{i'_\ell})$. Prove that $\sum_{i \in I} q_i \in -\bar{V}_{+,m}$ and $\sum_{i \in I'} q_i \in \bar{V}_{+,m}$.

147. Prove Theorem XI.117 in the notes for scattering on C^*-algebras.

148. (a) With the notation of Theorem XI.114, show that

$$N^{-1}\sum_{n=0}^{N-1}|F(n)|^2 \to \sum_{x\in\mathbf{R}}|\mu(\{x\})|^2 \qquad \text{as} \quad N\to\infty$$

(b) Let U be a unitary operator on a separable Hilbert space and let $\{E_i\}_{i=1}^{M}$ ($M = 1, \ldots, \infty$) be its eigenvalues and P_i the corresponding eigenprojections. Show that for any vectors η, ψ,

$$\lim_{N\to\infty} N^{-1}\sum_{n=0}^{N-1}|(\eta, U^n\psi)|^2 = \sum |(\eta, P_i\psi)|^2$$

(c) Suppose that $U\varphi = \varphi$. Prove that

$$\lim_{N\to\infty} N^{-1}\sum_{n=0}^{N-1}|(\eta, U^n\psi) - (\eta, \varphi)(\varphi, \psi)| = 0$$

for all η, $\psi \in \mathscr{H}$ if and only if φ is the only eigenvector of U. (This is Theorem VII.14b.)

149. (a) Map $Q = \times_{n=1}^{\infty}\{-1, 1\}$ onto $[0, 1]$ by $Tx = \sum_{n=1}^{\infty} 3^{-n}(x_n + 1)$. Put the measure $\mu_0(\{1\}) = \mu_0(\{-1\}) = \frac{1}{2}$ on $\{-1, 1\}$ and the product measure μ on Q. Define ν on $[0, 1]$ by $\nu(A) = \mu(T^{-1}(A))$. Show that ν is the Cantor measure.

(b) Using (a), show that $F(t) = \int e^{ixt}\, d\nu(x)$ with ν the Cantor measure is given by

$$F(t) = e^{it/2}\prod_{n=1}^{\infty}\cos(3^{-n}t)$$

(c) Show that $F(3^N(2\pi))$ does not go to zero as $N \to \infty$ and conclude that $F(t) \not\to 0$ as $t \to \infty$.

(d) Let A be multiplication by x on $L^2(0, 1; d\nu)$. Show that $U(t) = e^{itA}$ does not go weakly to zero.

(e) If one maps Q onto $[0, 1]$ by $Sx = \sum_{n=1}^{\infty} 2^{-n-1}(x_n + 1)$, then $\nu(\cdot) = \mu(S^{-1}(\cdot))$ is just Lebesgue measure on $[0, 1]$. Why cannot one claim that $\tilde{F}(2^N(2\pi))$ does not go to zero?

(f) Prove that $t^{-1}\sin t = \prod_{n=1}^{\infty}\cos(2^{-n-1}t)$.

150. In the context of the Lax–Phillips theory suppose that one knows only that A_1 has purely continuous spectrum. Use Lemma 3 before Theorem XI.8 and the RAGE theorem to show that (219) holds.

151. Let V be H_0($= -\frac{1}{2}\Delta$)-bounded and pick a fixed j with $1 - j \in C_0^{\infty}$, $j(x) = 1$ (respectively, 0) if $|x| \geq 1$ (respectively, $|x| \leq \frac{1}{2}$). Let $j_R(x) = j(x/R)$. For $z \notin \sigma(H_0)$, let

$$h(R, z) = \|V(H_0 - z)^{-1}F(|x| \geq R)\|,$$

$$h_1(R, z) = \|V(H_0 - z)^{-1}j_R\|, \qquad h_2(R, z) = \|Vj_R(H_0 - z)^{-1}\|.$$

(a) Prove that $h(R, z) \leq h_1(R, z) \leq h(\frac{1}{2}R, z)$ and conclude that $h \in L^1(0, \infty; dR)$ if and only if $h_1 \in L^1$ for the same z.

(b) Use a commutator to prove that

$$|h_1(R) - h_2(R)| \leq C_z R^{-1}h_1(\tfrac{1}{2}R)$$

and prove that $h_1 \in L^1$ if and only if $h_2 \in L^1$ for the same z.

(c) Use the first resolvent formula to show that the condition $h_2 \in L^1$ is z-independent.
(d) Let V commute with each j_R. Prove that $h(R, z)$ is in L^1 if and only if $\|F(|x| \geq R)V(H_0 - z)^{-1}\|$ is in L^1.

152. (a) Extend the formulas (270n, o, p) for the current to accommodate several components $\{u_\alpha\}_{\alpha=1}^n$ with the possibility that V mixes components.
(b) An **internal symmetry** has the form $y = x, s = t, V_\alpha$ is a function of $\{u_\beta\}$ alone. Write a formula for the conserved quantity resulting from an internal symmetry.
(c) Let $\mathscr{L}(u) = |u_t|^2 - |\nabla u|^2 - G(u)$. Suppose that u is allowed to be complex-valued but that G is only a function of $|u|$. Find the conserved quantity Q (the conventional "charge") corresponding to the internal symmetry $u \to e^{i\varepsilon}u$.
(d) Let u be an n-component function and let $\mathscr{L}(u) = |u_t|^2 - |\nabla u|^2 - G(u)$. If $\mathscr{L}$ is a function only of $|u|$, write down the conserved quantities in case u is real-valued ($O(n)$-symmetry) or complex-valued ($U(n)$ symmetry). Suppose that $\mathscr{L}$ has a symmetry breaking term $-F(u_1)$ added to it. Compute the sources now introduced into the previously conserved currents.

153. (a) For the equation $u_{tt} = \Delta u - |u|^{p-1}u$, let k_0 be given by (270d) with $\frac{1}{4}u^4$ replaced by $(1/p + 1)|u|^{p+1}$. Find the source term in the corresponding broken conformal invariance.
(b) If $p > 3$, show that $S(u) \leq 0$ for $t > 0$.
*(c) For $3 < p < 5$, prove the analogue of Theorem XI.101.

154. Suppose that $\mathscr{L}(u)$ has the form $\partial_0 B_0 + \nabla \cdot \mathbf{B}$ for some local functions B_0, $\mathbf{B}$ of u. Show that every function obeys the corresponding Euler–Lagrange equations.

155. Find the other nine conserved quantities for (270b), i.e., the six Lorentz invariance charges and the other three conformal charges.

156. (a) Find the dilation current and source term for $u_{tt} = \Delta u - |u|^{p-1}u$ when $x \in \mathbb{R}^n, t \in \mathbb{R}$. Choose the transformation law on u such that $\delta\mathscr{L} = 0$ for the "free" case $u_{tt} = \Delta u$.
(b) Repeat this for the conformal charge.

Material Preprinted from Volume IV

The crucial (and often hardest) step in most proofs of asymptotic completeness for quantum systems is the proof that the interacting Hamiltonian has no singular continuous spectrum. Conversely, one of the best ways of showing that a self-adjoint operator has no singular continuous spectrum is to show that it is the interaction Hamiltonian of a quantum system with complete wave operators. This deep connection between scattering theory and spectral analysis shows how artificial the division of material into Volumes III and IV really is. Therefore, as an aid to readers whose primary interest is scattering theory, we have preprinted below three sections from Volume IV.

XIII.6 The absence of singular continuous spectrum I: General theory

Spectral analysis of an operator A concentrates on identifying the five sets $\sigma_{\text{ess}}(A)$, $\sigma_{\text{disc}}(A)$, $\sigma_{\text{ac}}(A)$, $\sigma_{\text{sing}}(A)$, $\sigma_{\text{pp}}(A)$. For large classes of Schrödinger operators H, we have succeeded in identifying $\sigma_{\text{ess}}(H)$ and $\sigma_{\text{ac}}(H)$. A precise determination of $\sigma_{\text{disc}}(H)$ is a detailed question, but we have seen how to use the min–max principle to obtain a lot of information about it. That leaves $\sigma_{\text{sing}}(H)$ and $\sigma_{\text{pp}}(H)$. We shall discuss the question of proving $\sigma_{\text{pp}} = \sigma_{\text{disc}}$ in Section 13. The next five sections involve the difficult study of $\sigma_{\text{sing}}(H)$. Our discussion of asymptotic completeness in Section XI.3 suggests that $\sigma_{\text{sing}}(H) = \emptyset$ and our main goal will be the proof of this fact for various classes of Schrödinger operators.

As we have already emphasized, there are close connections between proving the absence of singular continuous spectrum and scattering theory. In fact, the development of eigenfunction expansions in Section XI.6 already tells us something about the singular spectrum. In general when $V \in L^1 \cap R$ we know that $\sigma_{\text{sing}} \subset \mathscr{E}$, the exceptional set, so that σ_{sing} has Lebesgue measure 0. And in two cases, first when $V \in L^1 \cap R$ and $\|V\|_R < 4\pi$, and secondly, if $Ve^{a|x|} \in R$ for some $a > 0$, we know that $\mathscr{E}$ is discrete so that $\sigma_{\text{sing}} = \emptyset$. In this section we shall develop a fundamental criterion for the absence of singular spectrum and show how it allows us to recover these two results from first principles without very much effort. In Sections 7 and 8, we shall use the connection between scattering theory and spectral analysis in reverse: The techniques developed to prove that there is no singular continuous spectrum will yield very strong results on asymptotic completeness.

The fundamental criterion for the absence of singular spectrum is very simple. In part it will depend on Stone's formula (Theorem VII.13):

$$\tfrac{1}{2}(\varphi, (E_{[a,b]} + E_{(a,b)})\varphi) = \lim_{\varepsilon \downarrow 0} \pi^{-1} \int_a^b \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

where $R(\lambda)$ is the resolvent $(H - \lambda)^{-1}$ of some self-adjoint H and $\{E_\Omega\}$ is its family of spectral projections. In particular, one has that

$$\sup_{0<\varepsilon<1} \int_a^b |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx < \infty \tag{30}$$

in the case $p = 1$ for any $\varphi \in \mathscr{H}$.

Theorem XIII.19 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval and $\varphi \in \mathscr{H}$. Suppose that there is a $p > 1$ for which (30) holds. Then $E_{(a,b)}\varphi \in \mathscr{H}_{ac}$.

Proof By Stone's formula and the fact that $E_{(c,d)} \leq E_{[c,d]}$

$$(\varphi, E_{(c,d)}\varphi) \leq \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \int_c^d \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx$$

for each open interval (c, d). Let S be an open set in (a, b) so that $S = \bigcup_{i=1}^{N} (a_i, b_i)$ is a union of disjoint open intervals. Suppose first that $N < \infty$. Then

$$\begin{aligned}(\varphi, E_S\varphi) &\le \frac{1}{\pi} \sum_{i=1}^{N} \lim_{\varepsilon \downarrow 0} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx \\ &\le \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \sum_{i=1}^{N} \int_{a_i}^{b_i} \operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)\, dx \\ &\le \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \left[\int_a^b |\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi)|^p\, dx\right]^{1/p} |S|^{1/q} \\ &\le C|S|^{1/q}\end{aligned}$$

where $|S|$ is the Lebesgue measure of S and q is the conjugate index to p. If N is infinite, let $S_m = \bigcup_{i=1}^{m} (a_i, b_i)$. Then

$$(\varphi, E_S\varphi) = \lim_{m\to\infty} (\varphi, E_{S_m}\varphi) \le \lim_{m\to\infty} C|S_m|^{1/q} = C|S|^{1/q}$$

Let I be an arbitrary set of Lebesgue measure 0 inside (a, b). Since Lebesgue measure is outer-regular, we can find an open set $S^{(k)}$ with $I \subset S^{(k)}$ and $|S^{(k)}| < 1/k$. Thus

$$(\varphi, E_I\varphi) \le \inf_k (\varphi, E_{S^{(k)}}\varphi) \le C \inf_k |S^{(k)}|^{1/q} = 0$$

Thus the measure $\Omega \mapsto (\varphi, E_\Omega\varphi)$ is absolutely continuous on (a, b) so $E_{(a,b)}\varphi \in \mathscr{H}_{\text{ac}}$. ▌

Theorem XIII.20 Let H be a self-adjoint operator with resolvent $R(\lambda) = (H - \lambda)^{-1}$. Let (a, b) be a bounded interval. Suppose that there is a dense set D in $\mathscr{H}$ so that, for each $\varphi \in D$, (30) holds for some $p > 1$. Then H has purely absolutely continuous spectrum on (a, b), i.e., $\operatorname{Ran} E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$. Conversely, if $\operatorname{Ran} E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$, then there is a set D, dense in $\operatorname{Ran} E_{(a,b)}$, so that (30) holds for any $p \ge 1$ including $p = \infty$ when $\varphi \in D$.

Proof The first half of the theorem follows from Theorem XIII.19. For the second half, let D be the set of vectors φ for which the spectral measure $d\mu_\varphi$ for H is of the form $f(x)\, dx$ where $f \in L^\infty$ with compact support in (a, b). By hypothesis, D is dense in $\operatorname{Ran} E_{(a,b)}$. Moreover,

$$\operatorname{Im}(\varphi, R(x + i\varepsilon)\varphi) = \int_{-\infty}^{\infty} g_\varepsilon(x - y) f(y)\, dy$$

where $g_\varepsilon(y) = \varepsilon(y^2 + \varepsilon^2)^{-1}$. Since $\|g_\varepsilon\|_1 = \pi$ independently of ε, (30) holds with $p = \infty$ by Young's inequality and thus for all p since (a, b) is finite. ▌

In most applications of Theorem XIII.20, one actually proves that $(\varphi, R(\lambda)\varphi)$ is bounded on $M = \{x + i\varepsilon \mid \varepsilon \in (0, 1), x \in (a, b)\}$ or more strongly that $(\varphi, R(\lambda)\varphi)$ has a continuous extension to $\bar{M}$. A typical application is:

Theorem XIII.21 Let $V \in R$, the Rollnik class, and let $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$. Suppose that *either*:

(a) $\|V\|_R < 4\pi$;

or

(b) $Ve^{a|x|} \in R$ for some $a > 0$.

Then $\sigma_{\text{sing}}(H) = \varnothing$.

Proof (a) Since $\|V\|_R < 4\pi$, $|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}$ has a Hilbert–Schmidt norm less than one uniformly for $\lambda \in \mathbb{C}\backslash[0, \infty)$ (see Section XI.6). Let $f \in C_0^\infty$ and note that $|f|^{1/2} \in R$. Then

$$\begin{aligned} |f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & + \sum_{n=0}^{\infty} (-1)^{n+1}(|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^n \\ & \times (|V|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2}) \end{aligned}$$

converges uniformly in Hilbert–Schmidt norm to an operator with norm less than $C_1 + C_2(1 - (4\pi)^{-1}\|V\|_R)^{-1}$. Thus

$$|(f, (H - \lambda)^{-1}f)| \le \| \, |f|^{1/2} \|_2 \, \| \, |f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} \|$$

is bounded on $\mathbb{C}\backslash[0, \infty)$. The fundamental criterion, Theorem XIII.19, thus implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ for *all* (a, b) so σ_{pp} and σ_{sing} are empty.

(b) As in our discussion in Section XI.6, $(1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}$ exists for all $\lambda \in \mathbb{C}\backslash[0, \infty)$ and has continuous boundary values as $\lambda \to x + i0$ as long as x avoids a finite set $\mathscr{E}$ of real numbers. Let $[a, b]$ be disjoint from $\mathscr{E}$. Then

$$\begin{aligned} |f|^{1/2}(H - \lambda)^{-1}|f|^{1/2} = {} & |f|^{1/2}(H_0 - \lambda)^{-1}|f|^{1/2} \\ & - (|f|^{1/2}(H_0 - \lambda)^{-1}V^{1/2}) \\ & \times (1 + |V|^{1/2}(H_0 - \lambda)^{-1}V^{1/2})^{-1}|V|^{1/2} \\ & \times (H_0 - \lambda)^{-1}|f|^{1/2} \end{aligned}$$

is a uniformly bounded operator on $\{x + i\varepsilon \mid 0 < \varepsilon < 1; x \in [a, b]\}$ whenever $f \in C_0^\infty$. As in (a), this implies that Ran $E_{(a,b)} \subset \mathscr{H}_{\text{ac}}$ so $\sigma_{\text{sing}} \subset \mathscr{E}$, a finite set. This implies that $\sigma_{\text{sin}} = \varnothing$. ∎

Given the simple criterion, Theorem XIII.20, for $\sigma_{\text{sing}}(H)$ to be empty, one can reasonably ask why the problem of controlling the singular continuous spectrum is so much more difficult than that of identifying $\sigma_{\text{ess}}(H)$ (Sections 4 and 5) or $\sigma_{\text{ac}}(H)$ (Section XI.3). The reason is that σ_{sing} is much less stable under perturbations. To illustrate this, we describe the Aronszajn–Donoghue theory of the behavior of σ_{sing} under rank one perturbations. This theory should be compared with the Weyl theorem on invariance of σ_{ess} and the Kato–Birman theory of the invariance of σ_{ac}. Basic to the Aronszajn–Donoghue theory is the following combination of classical results of Fatou and de la Vallée Poussin:

Proposition Let ν be a finite Borel measure on $\mathbb{R}$ and let

$$F(z) = \int (x - z)^{-1}\, d\nu(x)$$

for $\operatorname{Im} z > 0$. Let $A_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \infty\}$ and let

$$B_\nu = \{x \mid \lim_{\varepsilon \downarrow 0} F(x + i\varepsilon) = \Phi(x), \text{ a finite number with } \operatorname{Im} \Phi(x) \neq 0\}$$

Then $\nu(\mathbb{R}\backslash(A_\nu \cup B_\nu)) = 0$, $\nu \restriction A_\nu$ is singular relative to Lebesgue measure, and $\nu \restriction B_\nu$ is absolutely continuous.

Proofs of this result may be tracked down by consulting the reference in the notes. Now let H_0 be some self-adjoint operator on $\mathscr{H}$ and let $\varphi \in \mathscr{H}$ be a unit vector. Let P denote the projection onto φ and let

$$H_\alpha = H_0 + \alpha P$$

Let $\mathscr{H}'$ be the cyclic subspace for φ generated by H_0. Clearly all the H_α equal H_0 on $(\mathscr{H}')^\perp$ so we may as well suppose that $\mathscr{H}' = \mathscr{H}$, that is, we henceforth suppose that φ is cyclic for H_0. It follows that φ is also cyclic for H_α since

$$(H_\alpha - z)^{-1}\varphi = (H_0 - z)^{-1}\varphi - \alpha(\varphi, (H_0 - z)^{-1}\varphi)(H_\alpha - z)^{-1}\varphi$$

so that the span of $\{(H_\alpha - z)^{-1}\varphi\}$ is identical to the span of $\{(H_0 - z)^{-1}\varphi\}$. By this cyclicity result, H_α is unitarily equivalent to multiplication by x on $L^2(\mathbb{R}, d\nu_\alpha)$ for a suitable measure $d\nu_\alpha$.

Clearly,

$$F_\alpha(z) \equiv \int (x - z)^{-1}\, d\nu_\alpha(x) = (\varphi, (H_\alpha - z)^{-1}\varphi)$$

obeys

$$F_\alpha(z) = F_\beta(z) + (\beta - \alpha)F_\alpha(z)F_\beta(z)$$

on account of the resolvent equation

$$(H_\alpha - z)^{-1} = (H_\beta - z)^{-1} + (\beta - \alpha)(H_\alpha - z)^{-1}P(H_\beta - z)^{-1}$$

Thus, we have the basic equation:

$$F_\alpha(z) = F_\beta(z)(1 + (\alpha - \beta)F_\beta(z))^{-1} \tag{30.5}$$

Note that if $\lim_{\varepsilon \downarrow 0} F_\beta(z) = \infty$, then $\lim_{\varepsilon \downarrow 0} F_\alpha(z) = (\alpha - \beta)^{-1} \neq \infty$ for $\alpha \neq \beta$. Applying the proposition, we have proven the following striking *noninvariance* of σ_{sing}:

Theorem XIII.21.5 Let H_0 be a self-adjoint operator and let φ be a cyclic vector for H_0. Let

$$H_\alpha = H_0 + \alpha(\varphi, \cdot)\varphi$$

Then for $\alpha \neq \beta$ the singular (i.e., the union of pure point and singular continuous) parts of the spectral measures for H_α and H_β are mutually singular.

Example Let $d\nu_0 = dx \restriction [0, 1] + d\mu_C$, where $d\mu_C$ is the Cantor measure. Then $\sigma_{\text{ess}}(H_\alpha) = [0, 1]$ for all α on account of Weyl's theorem. Moreover, $F_0 = F_L + F_C$ in the obvious way, and

$$\lim_{\varepsilon \downarrow 0} \operatorname{Im} F_L(x + i\varepsilon) = \begin{cases} 1, & x \in (0, 1) \\ \frac{1}{2}, & x = 0, 1 \\ 0, & x \notin [0, 1] \end{cases}$$

Since $\operatorname{Im} F_C(z) \geq 0$ for all z with $\operatorname{Im} z > 0$, we see that $\lim_{\varepsilon \downarrow 0} F_0(x + i\varepsilon)$ is never real for any $x \in [0, 1]$. It follows from the basic equation (30.5) that $\lim_{\varepsilon \downarrow 0} F_\beta(x + i\varepsilon)$ is never infinite for $\beta \neq 0$, $x \in [0, 1]$. Thus, each H_β for $\beta \neq 0$ has no singular continuous spectrum while $\sigma_{\text{sing}}(H_0) \neq \emptyset$. Thus, we have two bounded operators H_0 and H_1 such that $H_0 - H_1$ has rank one, with $\sigma_{\text{sing}}(H_1) = \emptyset \neq \sigma_{\text{sing}}(H_0)$!

XIII.7 The absence of singular continuous spectrum II: Smooth perturbations

Theorem XIII.20 suggests that one study L^p bounds on expectation values of the resolvent and our experience suggests that $p = 2$ will be particularly easy to study.

Definition Let H be a self-adjoint operator with resolvent $R(\mu) = (H - \mu)^{-1}$. Let A be a closed operator. A is called **H-smooth** if and only if for each $\varphi \in \mathscr{H}$ and each $\varepsilon \neq 0$, $R(\lambda + i\varepsilon)\varphi \in D(A)$ for almost all $\lambda \in \mathbb{R}$ and moreover

$$\|A\|_H^2 = \sup_{\substack{\|\varphi\| = 1 \\ \varepsilon > 0}} \frac{1}{4\pi^2} \int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2)\, d\lambda < \infty \quad (31)$$

Since A is closed, it is enough that (31) hold for a dense set of φ (Problem 47a). More interestingly, the uniform boundedness principle shows that if for *each* φ, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2\, d\lambda \leq M_\varphi^2$ for a constant M_φ (independent of $\varepsilon > 0$ and of $\pm$, but dependent on φ), then A is H-smooth (Problem 47b,c).

The H-smooth operators are an especially nice class of operators. For example, we shall see that they are H-bounded with relative bound 0. They present in microcosm the close connection between scattering theory and spectral analysis. On one hand, we shall prove a basic result on the existence and completeness of wave operators $\Omega^\pm(H_1, H_0)$ when $H_1 - H_0$ is the product of an H_1-smooth operator and an H_0-smooth operator (Theorem XIII.24; see also Theorem XIII.31). On the other hand, we will see that if A is H-smooth, then $\overline{\operatorname{Ran}(A^*)} \subset \mathscr{H}_{\mathrm{ac}}(H)$ (Theorem XIII.23), which will lead to several theorems on the absence of singular continuous spectrum (see Theorems XIII.26 and XIII.28).

This section is divided into two parts. First, we shall develop the abstract theory of smooth perturbations, and in the second part we apply the theory to a variety of Schrödinger operators. The first two applications involve situations where the wave operators are unitary, i.e., where H and H_0 are unitarily equivalent. These are the cases of Schrödinger operators $H_0 + \lambda V$ with λ small or V repulsive. In the latter case, the theory of smooth perturbations will lead only to a proof that H has purely absolutely continuous spectrum. In our last application we shall establish the existence of wave operators for the case of repulsive potentials with some fall-off hypotheses by developing a generalization of the notion of H-smoothness. Part of this generalized theory will play a role in the next section.

One of our first main goals will be the reformulation of H-smoothness in a number of equivalent forms. We shall need the following vector-valued version of the Plancherel theorem.

Lemma 1 Let $\varphi(\cdot)$ be a (weakly measurable) function from $\mathbb{R}$ to a separable Hilbert space $\mathscr{H}$. Suppose that $\int \|\varphi(x)\|\, dx < \infty$. Define $\hat{\varphi}\colon \mathbb{R} \to \mathscr{H}$ by

$$\hat{\varphi}(p) = (2\pi)^{-1/2} \int_{\mathbb{R}} e^{-ipx}\varphi(x)\, dx$$

(where, by our standard convention, the integral is a weak integral). Let A be a closed operator on $\mathscr{H}$. Then

$$\int \|A\hat{\varphi}(p)\|^2 \, dp = \int \|A\varphi(x)\|^2 \, dx \tag{32}$$

where the integrals in (32) are set equal to ∞ if $\hat{\varphi}(p)$ (respectively, $\varphi(x)$) is not in $D(A)$ almost everywhere.

Proof First suppose that A is bounded. Then for any $\psi \in \mathscr{H}$, $(\psi, A\hat{\varphi}(p)) = (A^*\psi, \hat{\varphi}(p))$ is the (ordinary) Fourier transform of $(A^*\psi, \varphi(x)) = (\psi, A\varphi(x))$, so by the Plancherel theorem

$$\int |(\psi, A\hat{\varphi}(p))|^2 \, dp = \int |(\psi, A\varphi(x))|^2 \, dx$$

(32) follows by summing over ψ in an orthonormal basis. Next let A be self-adjoint and let $\{E_\Omega\}$ be its family of spectral projections. Then $AE_{(-a,a)}$ is bounded so

$$\int \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 \, dp = \int \|AE_{(-a,a)}\varphi(x)\|^2 \, dx$$

Suppose that one of the integrals in (32) is finite—without loss suppose the right-hand side is finite. Then $\varphi(x) \in D(A)$ a.e. in x, so $\|AE_{(-a,a)}\varphi(x)\|^2$ converges monotonically to $\|A\varphi(x)\|^2$ as $a \to \infty$. Thus,

$$\int \lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 \, dp = \int \|A\varphi(x)\|^2 \, dx < \infty$$

In particular, $\lim_{a\to\infty} \|AE_{(-a,a)}\hat{\varphi}(p)\|^2 < \infty$ a.e. in p. It follows that $\hat{\varphi}(p) \in D(A)$ a.e. and (32) holds. Finally, let A be an arbitrary closed operator. By Theorem VIII.32, there is a self-adjoint operator $|A|$ with $D(|A|) = D(A)$ and $\| |A| \psi\| = \|A\psi\|$. Thus (32) follows from the case where A is self-adjoint. ∎

Example 1 Let $H = -i\, d/dx$ on $L^2(\mathbb{R})$ so that $(e^{-iHt}\varphi)(x) = \varphi(x - t)$. Let g be in $L^2(\mathbb{R})$ and let A be multiplication by g. By a change of variables, $\int |g(x)\varphi(x-t)|^2 \, dx \, dt = \|g\|_2^2 \|\varphi\|_2^2$ so, by Fubini's theorem, for any $\varphi \in L^2$, and almost all t, $e^{-iHt}\varphi \in D(A)$ and $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt = \|g\|_2^2 \|\varphi\|_2^2$. Fix $\varepsilon > 0$; then

$$\int_0^\infty e^{-\varepsilon t} e^{i\lambda t} e^{-iHt}\varphi \, dt = -iR(\lambda + i\varepsilon)\varphi$$

Thus, by the lemma

$$\int_{-\infty}^{\infty} \|AR(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t}\|Ae^{-itH}\varphi\|^2 \, dt$$

Using a similar computation for $\lambda - i\varepsilon$, we see that

$$\int_{-\infty}^{\infty} (\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2) \, d\lambda = 2\pi \int_{-\infty}^{\infty} e^{-2\varepsilon|t|}\|Ae^{-itH}\varphi\|^2 \, dt \tag{33}$$

(33) and the bound on $\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$ imply that g is H-smooth and $\|g\|_H = (2\pi)^{-1/2}\|g\|_2$.

Example 2 Let H be any self-adjoint operator and let $A = I$, the identity operator. Again, we use Lemma 1 to conclude that

$$\int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = 2\pi \int_0^{\infty} e^{-2\varepsilon t}\|e^{-itH}\varphi\|^2 \, dt = \pi\varepsilon^{-1}\|\varphi\|^2 \tag{34}$$

so that $\sup_{\varepsilon > 0} \int_{-\infty}^{\infty} \|R(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = \infty$ for any $\varphi \neq 0$. Thus I is never an H-smooth operator.

One reformulation of H-smoothness is in terms of the unitary group e^{itH}. As an immediate consequence of (33) we have:

Lemma 2 A is H-smooth if and only if for all $\varphi \in \mathscr{H}$, $e^{itH}\varphi \in D(A)$ for almost every $t \in \mathbb{R}$ and for some constant C,

$$\int_{-\infty}^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt \leq C\|\varphi\|^2$$

C can be chosen equal to $(2\pi)\|A\|_H^2$ and no smaller.

This lemma has several important consequences:

Theorem XIII.22 If A is H-smooth, then A is H-bounded with relative bound zero.

Proof Let $\psi \in D(A^*)$. By the resolvent formula

$$-i(A^*\psi, R(\lambda + i\varepsilon)\varphi) = \int_0^{\infty} (A^*\psi, e^{-iHt}\varphi)e^{i\lambda t}e^{-\varepsilon t} \, dt$$

Thus, by the Schwarz inequality

$$\begin{aligned}|(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 &\leq \frac{1}{2\varepsilon}\int_0^\infty |(A^*\psi, e^{-iHt}\varphi)|^2\,dt\\ &\leq \frac{1}{2\varepsilon}\|\psi\|^2\int_0^\infty \|Ae^{-iHt}\varphi\|^2\,dt\\ &\leq \frac{\pi}{\varepsilon}\|A\|_H^2\|\psi\|^2\|\varphi\|^2\end{aligned}$$

by Lemma 2. Thus, $R(\lambda + i\varepsilon)\varphi \in D(A^{**}) = D(A)$ and $\|AR(\lambda + i\varepsilon)\|^2 \leq (\pi/\varepsilon)\|A\|_H^2$. We conclude that $D(H) \subset D(A)$ and for $\psi \in D(H)$

$$\|A\psi\| \leq \pi^{1/2}\|A\|_H(\varepsilon^{-1/2}\|H\psi\| + \varepsilon^{1/2}\|\psi\|)$$

Since ε is arbitrary, the theorem is proven. ∎

For a strengthening of Theorem XIII.22, see Problem 49.

Theorem XIII.23 If A is H-smooth, then $\overline{\operatorname{Ran}(A^*)} \subset \mathscr{H}_{\mathrm{ac}}(H)$.

Proof Since $\mathscr{H}_{\mathrm{ac}}(H)$ is closed, we need only show $\operatorname{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$. Let $\varphi \in D(A^*)$, $\psi = A^*\varphi$, and let $d\mu_\psi$ be the spectral measure for H associated with ψ. Define

$$F(t) = (2\pi)^{-1/2}\int e^{-itx}\,d\mu_\psi(x) = (2\pi)^{-1/2}(A^*\varphi, e^{-itH}\psi)$$

Then $|F(t)| \leq (2\pi)^{-1/2}\|\varphi\|\,\|Ae^{-itH}\psi\|$, so by Lemma 2, $F \in L^2(\mathbb{R})$. By the Plancherel theorem, $\check{F} \in L^2$ so $d\mu_\psi = \check{F}\,dx$ is absolutely continuous with respect to Lebesgue measure. ∎

It is an instructive exercise to prove Theorem XIII.23 using Theorem XIII.20 and the direct definition of H-smoothness. See also condition (5) of Theorem XIII.25 below. Lemma 2 has important consequences for scattering theory.

Theorem XIII.24 Let H and H_0 be self-adjoint operators. Suppose that $H = H_0 + \sum_{i=1}^n A_i^*B_i$ in the following sense:

(1) $D(H) \subset D(A_i)$; $D(H_0) \subset D(B_i)$; $i = 1, \ldots, n$.

(2) If $\varphi \in D(H)$ and $\psi \in D(H_0)$, then

$$(H\varphi, \psi) = (\varphi, H_0\psi) + \sum_{i=1}^n (A_i\varphi, B_i\psi) \tag{35}$$

Corollary If $AR(\mu)A^*$ is bounded for each $\mu \notin \mathbb{R}$ in the sense that

$$\sup_{\substack{\psi,\,\varphi \in D(A^*)\\ \|\psi\| = \|\varphi\| = 1}} |(A^*\varphi, R(\mu)A^*\psi)| < \infty \qquad \text{and} \qquad \Gamma \equiv \sup_{\mu \notin \mathbb{R}} \|AR(\mu)A^*\| < \infty$$

then A is H-smooth and $\|A\|_H \le \Gamma/\pi$.

Proof of Theorem XIII.25 We first note that for every closed operator A, every bounded operator B, every $\varphi \in D(A)$, and $\psi \in \mathscr{H}$, we have

$$(\psi, BA\varphi) = (B^*\psi, A\varphi)$$

It follows that $\|BA\varphi\| \le c\|\varphi\|$ for all $\varphi \in D(A)$ if and only if Ran $B^* \subset D(A^*)$ and $\|A^*B^*\| \le c$. As a consequence $c_2 = c_3$ and $c_5 = c_6$. Moreover, since $(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi) = 2 \operatorname{Im} \mu \|R(\mu)A^*\varphi\|^2$, $c_5 = c_4$. Further, $c_0 = c_1$ by Lemma 2. Thus we need only prove that $c_0 = c_3 = c_4 = c_7$ where $c_0 \equiv \|A\|_H^2$. We shall show that

$$c_0 \le c_4 \le c_3 \le c_0 \qquad \text{and} \qquad c_3 \le c_7 \le c_1 .$$

$c_0 \le c_4$: $(2\pi i)^{-1}[R(\mu) - R(\bar{\mu})] = \pi^{-1}(\operatorname{Im} \mu)R(\bar{\mu})R(\mu) \ge 0$ if $\operatorname{Im} \mu > 0$. Let $K(\mu)$ be its positive square root. By the definition of c_4, $\|K(\mu)A^*\varphi\|^2 \le c_4\|\varphi\|^2$ if $\varphi \in D(A^*)$. Thus, if $c_4 < \infty$, the remark above implies that Ran $K(\mu) \subset D(A)$ and $\|AK(\mu)\|^2 \le c_4$. Therefore

$$\begin{aligned}
&\int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda \\
&\qquad = 4\pi^2 \int_{-\infty}^{\infty} \|AK(\lambda + i\varepsilon)K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda \\
&\qquad \le 4\pi^2 c_4 \int_{-\infty}^{\infty} \|K(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda \\
&\qquad = 4\pi^2 c_4 \frac{1}{2\pi i} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda \\
&\qquad = 4\pi^2 c_4 \|\varphi\|^2
\end{aligned}$$

since in terms of the spectral measure $d\mu_\varphi$ for H,

$$\begin{aligned}
&(2\pi i)^{-1} \int_{-\infty}^{\infty} (\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi) \, d\lambda \\
&\qquad = \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(x - \lambda)^2 + \varepsilon^2} \, d\mu_\varphi(x) \, d\lambda \\
&\qquad = \int_{-\infty}^{\infty} d\mu_\varphi(x) = \|\varphi\|^2
\end{aligned}$$

Further,

$$[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi = i \int_{-\infty}^{\infty} e^{-\varepsilon|t|} e^{i\lambda t} e^{-iHt}\varphi \, dt$$

so Lemma 1 implies that

$$\int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\varphi\|^2 \, d\lambda = 2\pi \int_{-\infty}^{\infty} e^{-2\varepsilon|t|} \|Ae^{-iHt}\varphi\|^2 \, dt \tag{36}$$

so $c_0 = c_1 \le c_4$.

$c_4 \le c_3$: Let $\varphi \in D(A^*)$ and let $d\mu_{A^*\varphi}$ be the spectral measure for H with respect to $A^*\varphi$. Then, by (3)

$$d\mu_{A^*\varphi}(a, b] \le c_3 |b - a| \, \|\varphi\|^2$$

If I is an arbitrary Borel set, let $|I|$ be its Lebesgue measure. It follows that $d\mu_{A^*\varphi}(I) \le c_3 |I| \, \|\varphi\|^2$ for arbitrary I, for it is true for open sets and thus by outer regularity for arbitrary sets. Therefore $d\mu_{A^*\varphi}$ is absolutely continuous w.r.t. dx and the Radon–Nikodym derivative $g(x)$ obeys $\|g\|_\infty \le c_3 \|\varphi\|^2$. Thus if $\mu = \lambda + i\varepsilon$, then

$$\begin{aligned} |(A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi)| &= \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} g(x) \, dx \\ &\le \|g\|_\infty \int_{-\infty}^{\infty} \frac{2|\varepsilon|}{(x - \lambda)^2 + \varepsilon^2} \, dx \le c_3(2\pi)\|\varphi\|^2 \end{aligned}$$

We conclude that $c_4 \le c_3$.

$c_3 \le c_0$: Let $\varphi \in D(A^*)$. Suppose that a and b are not eigenvalues of H. By Stone's formula,

$$\begin{aligned} &|(A^*\varphi, E_{(a,b]}\psi)|^2 \\ &\quad = \frac{1}{4\pi^2} \lim_{\varepsilon \downarrow 0} \left| \int_a^b (A^*\varphi, [R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi) \, d\lambda \right|^2 \\ &\quad \le \frac{1}{4\pi^2} \|\varphi\|^2 \, |b - a| \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\infty} \|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]\psi\|^2 \, d\lambda \\ &\quad \le |b - a| \, \|A\|_H^2 \, \|\varphi\|^2 \, \|\psi\|^2 \end{aligned}$$

In the last step we have used (36). If a and/or b are eigenvalues, $a + \delta$ and $b + \delta$ are not eigenvalues for almost all small δ and $E_{(a,b]} = \text{s-lim}_{\delta \to 0} E_{(a+\delta, b+\delta]}$ so we see that $c_3 \le c_0$.

$c_3 \le c_7$: We already know that $c_3 = c_6$, and $c_6 \le c_7$ is obvious.

$c_7 \le c_1$: This is essentially the argument used in the proof of Theorem XIII.22. For by that argument,

$$|(A^*\psi, R(\lambda + i\varepsilon)\varphi)|^2 \le \frac{1}{2\varepsilon} \|\psi\|^2 \int_0^{\infty} \|Ae^{-iHt}\varphi\|^2 \, dt$$

so

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 \le \frac{1}{2\varepsilon} \int_0^\infty \|Ae^{-iHt}\varphi\|^2 \, dt$$

A similar argument for $R(\lambda - i\varepsilon)$ proves that

$$\|AR(\lambda + i\varepsilon)\varphi\|^2 + \|AR(\lambda - i\varepsilon)\varphi\|^2 \le \frac{1}{2\varepsilon} \int_{-\infty}^\infty \|Ae^{-iHt}\varphi\|^2 \, dt$$

Thus $c_7 \le c_1$. ▌

Notice that criterion (3) provides another proof that $\operatorname{Ran}(A^*) \subset \mathscr{H}_{\mathrm{ac}}(H)$ if A is H-smooth, and that criterion (6) implies Theorem XIII.22. The equality of c_6 and c_7 at first sight seems very mysterious. Some of this mystery can be removed by looking at the proof of a closely related equality:

$$\sup_{\substack{\varepsilon > 0 \\ \|\varphi\| = 1}} \int_{-\infty}^\infty \|AR(\lambda + i\varepsilon)\varphi\|^2 \, d\lambda = \sup_{\substack{\varepsilon > 0 \\ \|\varphi\| = 1}} \left\{ \int_{-\infty}^\infty (\|AR(\lambda + i\varepsilon)\varphi\|^2 \right.$$
$$\left. + \|AR(\lambda - i\varepsilon)\varphi\|^2) \, d\lambda \right\}$$

By (33), this equality is equivalent to

$$\sup_{\|\varphi\| = 1} \int_0^\infty \|Ae^{-itH}\varphi\|^2 \, dt = \sup_{\|\varphi\| = 1} \int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2 \, dt$$

which follows by noting that if $\varphi_s = e^{-isH}\varphi$, then

$$\int_0^\infty \|Ae^{-itH}\varphi_s\|^2 \, dt = \int_s^\infty \|Ae^{-itH}\varphi\|^2 \, dt$$

converges to $\int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2 \, dt$ as $s \to -\infty$.

Before turning to applications, we give two more examples of smooth operators:

Example 3 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and let A be multiplication by $V \in R$, the Rollnik class. By the estimate,

$$\| \, |V|^{1/2}(H_0 - \lambda)^{-1} |V|^{1/2} \|_{\mathrm{oper}} \le \| \, |V|^{1/2}(H_0 - \lambda)^{-1} |V|^{1/2} \|_2$$
$$\le (4\pi)^{-1} \|V\|_R$$

and the corollary to Theorem XIII.25, $|A|^{1/2}$ is H-smooth.

Example 4 Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Let A be a bounded operator on $\mathscr{H}$ so that A^*A is an integral operator of the form

$$(A^*A\psi)(x) = \int_\alpha^\beta K(x, y)\psi(y)\, dy \tag{37}$$

with $\|K\|_\infty \equiv \operatorname{ess\,sup}_{[\alpha, \beta] \times [\alpha, \beta]} |K(x, y)| < \infty$. Then A is H-smooth with $\|A\|_H \le \|K\|_\infty^{1/2}$. For, let $(a, b]$ be an interval and $\|\varphi\| = 1$. Then

$$\begin{aligned}
\|AE(a, b]\varphi\|^2 &= (\varphi, E(a, b]A^*AE(a, b]\varphi) \\
&= \int_a^b \int_a^b K(x, y)\overline{\varphi(x)}\varphi(y)\, dx\, dy \\
&\le \left(\int_a^b \int_a^b |K(x, y)|^2\, dx\, dy\right)^{1/2} \left(\int_a^b \int_a^b |\bar{\varphi}(x)\varphi(y)|^2\, dx\, dy\right)^{1/2} \\
&\le |b - a|\, \|K\|_\infty\, \|\varphi\|^2
\end{aligned}$$

By criterion (2), $\|A\|_H \le \|K\|_\infty^{1/2}$. By further analysis (Problems 50, 51) one can show that for every H-smooth operator A, A^*A is of the form (37) and that $\|A\|_H = \|K\|_\infty^{1/2}$. In particular, we note that the analysis above shows that any integral operator

$$(A\psi)(x) = \int_\alpha^\beta A(x, y)\psi(y)\, dy$$

with $\|A\|_\infty < \infty$ is H-smooth. We have thus found many H-smooth operators and, in particular, H-smooth operators A with $\operatorname{Ker}(A) = \{0\}$. Example 1 is related to this example although the operator H in Example 1 is not bounded. For if $f \in L^2$, then $A =$ multiplication by f has $A^*A =$ multiplication by $g \equiv |f|^2 \in L^1$. Passing to the representation in which $-i\, d/dx$ is diagonal (by using Fourier transform), A^*A is an integral operator with kernel equal to $(2\pi)^{-1/2}\hat{g}(x - y) \in L^\infty$.

We turn now to various applications:

A. Weakly coupled quantum systems

Suppose that H_0 is a positive self-adjoint operator and that C is self-adjoint. If $|C|^{1/2}(H_0 + I)^{-1}|C|^{1/2}$ is a bounded operator with bound a, then for any $\varphi \in D(|C|^{1/2})$, $\|(H_0 + I)^{-1/2}|C|^{1/2}\varphi\|^2 \le a\|\varphi\|^2$ so

$(H_0 + I)^{-1/2}|C|^{1/2}$ is bounded. Taking adjoints, $Q(H_0) \subset Q(C)$ and $\| |C|^{1/2}(H_0 + I)^{-1/2}\|^2 \leq a$. It follows that $(\varphi, |C|\varphi) \leq a(\varphi, (H_0 + I)\varphi)$ for all $\varphi \in Q(H_0)$. Thus C is H_0-form bounded and if $a < 1$, the form sum $H = H_0 + C$ is self-adjoint. Such form sums are the subject of the following theorem.

Theorem XIII.26 (Kato's smoothness theorem) Let H_0 be a positive self-adjoint operator on a Hilbert space $\mathscr{H}$ and let $C_1, \ldots, C_n$ be self-adjoint operators with

$$\alpha_{ij} \equiv \sup_{\mu \notin \mathbb{R}} \| |C_i|^{1/2}(H_0 - \mu)^{-1}|C_j|^{1/2}\| < \infty$$

Suppose that $\{\alpha_{ij}\}_{1 \leq i, j \leq n}$ is the matrix of an operator of norm less than 1 on $\mathbb{C}^n$ (with the natural Hilbert space norm). Then:

(a) The form sum $H = H_0 + \sum_{i=1}^n C_i$ is a closed form on $Q(H_0)$.
(b) The wave operators $\text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

In particular, H and H_0 are unitarily equivalent operators.

Proof Introduce the Hilbert space $\mathscr{H}' = \bigoplus_{i=1}^n \mathscr{H}_i$ where each $\mathscr{H}_i$ is a copy of $\mathscr{H}$. By the discussion preceding the theorem and the hypothesis $\alpha_{ii} < \infty$, we have that each $|C_i|$ is H_0-form bounded, so that $|C_i|^{1/2}$ is defined from $Q(H_0)$ to $\mathscr{H}$. As a result, we can define B: $Q(H_0) \to \mathscr{H}'$ by $(B\psi)_i = |C_i|^{1/2}\psi$. The hypothesis of the theorem implies that

$$\alpha \equiv \sup_{\mu \notin \mathbb{R}} \|B(H_0 - \mu)^{-1}B^*\| < 1 \tag{38}$$

Let $B = U|B|$ be the polar decomposition of B. Then, since $|B| = U^*B$ and U is a partial isometry, (38) implies that $|B|(H_0 + I)^{-1}|B|$ is a bounded operator of norm smaller than α. Again, it follows from the argument preceding the theorem that

$$(\varphi, |B|^2\varphi) \leq \alpha(\varphi, (H_0 + I)\varphi)$$

or that

$$\left(\varphi, \sum_{i=1}^n |C_i|\varphi\right) \leq \alpha(\varphi, (H_0 + I)\varphi) \tag{39}$$

From (39), we conclude that $\sum_{i=1}^n C_i$ is H_0-form bounded with relative bound $\alpha < 1$ proving (a).

Next, we note that for $\mu \notin [0, \infty)$,

$$(H-\mu)^{-1} = (H_0-\mu)^{-1} - \sum_{n=0}^{\infty} (-1)^n (H_0-\mu)^{-1} B^* W (B(H_0-\mu)^{-1} B^* W)^n B(H_0-\mu)^{-1} \tag{40}$$

where $W: \mathscr{H}' \to \mathscr{H}'$ by $(W\varphi)_i = (\operatorname{sgn} C_i)\varphi_i$. (40) holds since the sum is convergent by (38) and one checks that, in the language of quadratic forms (Section VIII.6), the right-hand side maps $\mathscr{H}_{-1}$ to $\mathscr{H}_{+1}$ and is an inverse for $(H-\mu): \mathscr{H}_{+1} \to \mathscr{H}_{-1}$. From (40) one easily sees that

$$\sup_{\mu \notin \mathbb{R}} \|B(H-\mu)^{-1}B^*\| \le \alpha(1-\alpha)^{-1} \tag{41}$$

so each $|C_i|^{1/2}$ and $C_i^{1/2} \equiv |C_i|^{1/2} \operatorname{sgn} C_i$ is H-smooth by the corollary to Theorem XIII.25. Similarly, by the basic hypotheses and that corollary, each $|C_i|^{1/2}$ is H_0-smooth. Thus, by Theorem XIII.24, both $\text{s-lim}_{t \to \mp\infty} e^{iHt}e^{-iH_0t}$ and $\text{s-lim}_{t \to \mp\infty} e^{iH_0t}e^{-iHt}$ exist. These maps are all isometries and inverses of one another. This proves (b). ▮

As an application of this theorem, the reader should prove the strong version of Theorem XIII.21 found in Problem 56. If one does not want to worry about detailed estimates, it is often useful to state Kato's smoothness theorem in the form:

Corollary Let H_0 be self-adjoint and positive. Let $C_1, \ldots, C_n$ be self-adjoint and let $C = \sum_{i=1}^n C_i$. Suppose that for each i and j

$$\sup_{\mu \notin \mathbb{R}} \| \, |C_i|^{1/2} (H_0-\mu)^{-1} |C_j|^{1/2} \| < \infty$$

Then there exists $\Lambda > 0$ so that for all $\lambda \in (-\Lambda, \Lambda)$:

(a) $H(\lambda) = H_0 + \lambda C$ is a closed form on $Q(H_0)$.
(b) The wave operators $\Omega_\lambda^\pm = \text{s-lim}_{t \to \mp\infty} e^{itH(\lambda)}e^{-itH_0}$ exist and are unitary.

It is actually possible to prove that $\Omega_\lambda^\pm$ are analytic in λ (see the Notes and Problems 53, 54). Now we can easily handle "weakly coupled" N-body Schrödinger operators.

Theorem XIII.27 (the Iorio–O'Carroll theorem) Let $m \geq 3$, $N \geq 2$. Let $\tilde{H}_0$ be the operator

$$\tilde{H}_0 = \sum_{i=1}^{N} (-2\mu_i)^{-1} \Delta_i$$

on $L^2(\mathbb{R}^{Nm})$ where each $\mu_i > 0$ and $r \in \mathbb{R}^{Nm}$ is written $r = \langle r_1, \ldots, r_N \rangle$ with $r_i \in \mathbb{R}^m$. Let H_0 be $\tilde{H}_0$ with the center of mass motion removed (see Section XI.5). Let $V = \sum_{i<j} V_{ij}(r_i - r_j)$ where each $V_{ij} \in L^{m/2+\varepsilon}(\mathbb{R}^m) \cap L^{m/2-\varepsilon}(\mathbb{R}^m)$ for some fixed $\varepsilon > 0$. Then for all $\lambda \in \mathbb{R}$ with $|\lambda|$ sufficiently small, $H_0 + \lambda V$ (defined as a form sum) is unitarily equivalent to H_0. The wave operators provide unitary equivalence. In particular, $H_0 + \lambda V$ has no bound states, no singular spectrum and has complete scattering.

Before proving the Iorio–O'Carroll theorem, we make several remarks. First, it is merely for contact with the notions of N-body quantum theory that we remove the center of mass motion. Secondly, we note that only when $m = 3$ is the form sum necessary. If $m \geq 4$, Theorem X.20 tells us that the operator sum $H_0 + \lambda V$ is self-adjoint on $C_0^\infty(\mathbb{R}m(N-1)$ if λ is real. Thirdly, we note that, by Theorem XIII.11, there can be no weak coupling theorem when $m = 1$ or 2, but there is a result on $L^2([0, \infty))$ (Problem 58). Finally, the conditions on V_{ij} cannot be weakened much; for if V_{ij} has non-$L^{m/2}$ local singularities at finite points (e.g., $r^{-2-\varepsilon}$ behavior at $r = 0$), then self-adjointness is lost and if V_{ij} has non-$L^{m/2}$ behavior at infinity (e.g., only $r^{-2+\varepsilon}$ falloff at ∞), then it can happen that $H_0 + \lambda V$ has bound states no matter how small λ is (see Theorem XIII.6).

Proof of Theorem XIII.27 Consider first the case $N = 2$. Then $H_0 = (-2\nu)^{-1} \Delta$ on $L^2(\mathbb{R}^m)$, so by Theorem IX.30,

$$\|e^{-iH_0t}\varphi\|_r \leq (ct)^{-m[\frac{1}{2}-r^{-1}]}\|\varphi\|_{r'} \tag{42}$$

where $2 \leq r \leq \infty$, $r^{-1} + r'^{-1} = 1$ and c is chosen suitably. Thus, if $f \in L^p$ and $p > 2$, then by Hölder's inequality and (42)

$$\|fe^{-iH_0t}f\varphi\|_2 \leq (ct)^{-mp^{-1}}\|f\|_p^2\|\varphi\|_2 \tag{43}$$

Thus, if $f \in L^{m-\varepsilon} \cap L^{m+\varepsilon}$ (and $m > 2 + \varepsilon$),

$$\int_{-\infty}^{\infty} \|fe^{-iH_0t}f\varphi\|_2 \, dt \leq d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2\|\varphi\|_2$$

for a suitable constant d. Since

$$f(H_0 - z)^{-1}f\varphi = i\int_0^{\infty} e^{izt}(fe^{-iH_0t}f)\varphi \, dt$$

if Im $z > 0$, we conclude that

$$\|f(H_0 - z)^{-1} f\varphi\|_2 \le d(\|f\|_{m+\varepsilon} + \|f\|_{m-\varepsilon})^2 \|\varphi\|_2$$

if Im $z > 0$. A similar argument holds if Im $z < 0$. Letting $f = |V|^{1/2}$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| |V|^{1/2}(H_0 - z)^{-1} |V|^{1/2}\| < \infty$$

The theorem (in case $N = 2$) then follows from the corollary to Theorem XIII.26.

To prove the theorem in the general case, we need only prove that

$$\sup_{z \notin \mathbb{R}} \| |V_{ij}|^{1/2}(H_0 - z)^{-1} |V_{k\ell}|^{1/2}\| < \infty$$

for all i, j, k, ℓ and apply the corollary to Theorem XIII.26. It is necessary to consider three distinct cases:

Case 1 $(ij) = (k\ell)$ Without loss of generality suppose that $i = k = 1$ and $j = \ell = 2$. Let $H_0^{(12)} = (-2\mu_{12})^{-1} \Delta_{12}$ where $\mu_{12}^{-1} = \mu_1^{-1} + \mu_2^{-1}$ and Δ_{12} is the Laplacian with respect to r_{12} in a Jacobi coordinate system (see Section XI.5). Thus, $H_0 - H_0^{(12)}$ depends only on the remaining Jacobi coordinates $\zeta_2, \ldots, \zeta_{N-1}$ and so commutes with any function of $\zeta_1 = r_2 - r_1$. If $f \in L^p(\mathbb{R}^m)$ and f_1 is multiplication by $f(\zeta_1)$, then

$$\|f_1 e^{-itH_0} f_1 \varphi\|_2 = \|f_1 e^{-itH_0^{(12)}} f_1 \varphi\|_2 \tag{44}$$

Let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. By the basic two-body estimate (43),

$$\int |f_1(e^{-iH_0^{(12)}t} f_1 \varphi(\zeta_1, \zeta_2, \ldots, \zeta_{N-1})|^2 \, d\zeta_1 \le (ct)^{-2mp^{-1}} \|f\|_p^4 \int |\varphi(\zeta)|^2 \, d\zeta_1$$

Integrating over $\zeta_2, \ldots, \zeta_{N-1}$ and using (44) we see that (43) still holds. Thus, by mimicking the two-body proof,

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2}(H_0 - z)^{-1} |V_{12}|^{1/2}\| < \infty$$

Case 2 $j = k$; i, j, ℓ distinct Without loss of generality, suppose that $i = 1$; $j = k = 2$; $\ell = 3$. Again use Jacobi coordinates with $\zeta_1 = r_2 - r_1$ and with $r_{23} = \alpha\zeta_1 + \beta\zeta_2$ (with $\alpha, \beta \neq 0$). Since $H_0 - H_0^{(12)}$ commutes with functions of ζ_1:

$$\| |V_{12}|^{1/2} e^{-itH_0} |V_{23}|^{1/2} \varphi\| = \| |V_{12}|^{1/2} e^{-itH_0^{(12)}} |V_{23}|^{1/2} \varphi\|$$

Fix $\zeta' \equiv \langle \zeta_2, \ldots, \zeta_{N-1} \rangle$ and let $\varphi \in \mathscr{S}(\mathbb{R}^{m(N-1)})$. Then by the basic two-body estimate (43),

$$\int |V_{12}(\zeta_1)| \, |e^{-itH_0^{(12)}} V_{23}^{1/2}(\alpha\zeta_1 - \beta\zeta_2)\varphi(\zeta_1, \zeta')|^2 \, d\zeta_1$$

$$\leq (ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \, \alpha^{-2m/p} \int |\varphi(\zeta)|^2 \, d\zeta_1$$

where we have used the fact that

$$\int |V_{23}(\alpha\zeta_1 - \beta\zeta_2)|^{p/2} \, d\zeta_1 = \alpha^{-1} \int |V_{23}(x)|^{p/2} \, dx$$

independently of ζ_2. Integrating over ζ', we find that

$$\| \, |V_{12}|^{1/2} e^{-itH_0^{(12)}} |V_{23}|^{1/2} \varphi\|_2^2 \leq \alpha^{-2/p} (ct)^{-2mp^{-1}} \|V_{12}\|_{p/2} \|V_{23}\|_{p/2} \|\varphi\|_2^2$$

From this estimate, it follows that

$$\sup_{z \notin \mathbb{R}} \| \, |V_{12}|^{1/2} (H_0 - z)^{-1} |V_{23}|^{1/2} \| < \infty$$

as in the two-body case.

Case 3 i, j, k, ℓ all distinct Without loss of generality suppose that $i = 1, j = 2, k = 3, \ell = 4$. Then,

$$\begin{aligned} &|(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2} \psi)| \\ &\quad = |(e^{+itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} |V_{34}|^{1/2} \psi)| \\ &\quad = |(|V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi, |V_{12}|^{1/2} e^{-it(H_0 - H_0^{(34)})} \psi)| \\ &\quad \leq \| \, |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi\| \, \| \, |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\| \end{aligned}$$

In the first step, we have used the fact that $|V_{12}|^{1/2}$ and $H_0^{(34)}$ commute; in the second step that $|V_{34}|^{1/2}$ commutes with $H_0 - H_0^{(34)}$ and $|V_{12}|^{1/2}$; and in the final step that $|V_{12}|^{1/2}$ and $H_0 - H_0^{(34)} - H_0^{(12)}$ commute. By step (1) and the corollary to Theorem XIII.25, $|V_{ij}|^{1/2}$ is $H_0^{(ij)}$-smooth. Thus,

$$\begin{aligned} &\int_{-\infty}^{\infty} \| \, |V_{34}|^{1/2} e^{+itH_0^{(34)}} \varphi\| \, \| \, |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\| \, dt \\ &\quad \leq \left(\int_{-\infty}^{\infty} \| \, |V_{34}|^{1/2} e^{itH_0^{(34)}} \varphi\|^2 \, dt \right)^{1/2} \\ &\quad \times \left(\int_{-\infty}^{\infty} \| \, |V_{12}|^{1/2} e^{-itH_0^{(12)}} \psi\|^2 \, dt \right)^{1/2} \\ &\quad \leq \| \, |V_{34}|^{1/2} \|_{H_0^{(34)}} \, \| \, |V_{12}|^{1/2} \|_{H_0^{(12)}} \, \|\varphi\| \, \|\psi\| \end{aligned}$$

so that

$$\int_{-\infty}^{\infty} |(\varphi, |V_{12}|^{1/2} e^{-itH_0} |V_{34}|^{1/2} \psi)| \, dt \le c\|\varphi\| \, \|\psi\|$$

Since

$$\begin{aligned}(\varphi, |V_{12}|^{1/2}(H_0 - z)^{-1} |V_{34}|^{1/2}\psi) \\ = -i \int_0^{\infty} e^{izt}(\varphi, |V_{12}|^{1/2} e^{-iH_0 t} |V_{23}|^{1/2}\psi) \, dt\end{aligned}$$

if Im $z > 0$, we conclude that

$$\sup_{z \notin \mathbb{R}} \| |V_{12}|^{1/2}(H_0 - z)^{-1} |V_{34}|^{1/2} \| < \infty$$

This completes the proof of case 3. ▮

If one of the particles has infinite mass, Case 2 cannot be handled as above since $\alpha = 0$ if $\mu_2 = \infty$. In that event, the method of case 3 will work and the theorem remains true.

B. Positive commutators and repulsive potentials

As a second application of smoothness techniques, we develop a method that will allow us to prove that Hamiltonians with repulsive potentials have purely absolutely continuous spectrum.

Theorem XIII.28 (the Putnam–Kato theorem) Let H and A be bounded self-adjoint operators. Suppose that $C = i[H, A]$ is positive. Then $C^{1/2}$ is H-smooth. In particular, if Ker $C = \{0\}$, then H has purely absolutely continuous spectrum.

Proof The second statement follows from the first by Theorem XIII.23 and the fact that $\text{Ker}(C^{1/2}) = [\text{Ran}(C^{1/2})]^{\perp} = \{0\}$. We compute:

$$\frac{d}{dt} e^{itH} A e^{-itH} \varphi = i e^{itH}[H, A] e^{-itH} \varphi = e^{itH} C e^{-itH} \varphi$$

Thus

$$\int_s^t (\varphi, e^{i\tau H} C e^{-i\tau H} \varphi) \, d\tau = (\varphi, e^{itH} A e^{-itH} \varphi) - (\varphi, e^{isH} A e^{-isH} \varphi)$$

so

$$\int_s^t \|C^{1/2}e^{-i\tau H}\varphi\|^2\,d\tau \le 2\|A\|\,\|\varphi\|^2$$

Since t and s are arbitrary, $C^{1/2}$ is H-smooth and

$$\|C^{1/2}\|_H^2 \le \|A\|/\pi \quad \blacksquare$$

For an alternative method of proof, see Problem 59.

Example 5 Since examples of positive commutators are not easy to construct directly, we present examples to show that the hypotheses of Theorem XIII.28 are sometimes obeyed. In fact, there is a sort of converse to the fact that $C^{1/2}$ is H-smooth: If H is bounded and B is any bounded H-smooth operator, there exists a bounded operator A with $i[H, A] = B^*B$. Since there are H-smooth operators with zero kernel when H has purely absolutely continuous spectrum (see Example 4), one can construct many pairs H, A for which the hypotheses of Theorem XIII.28 are obeyed. If B is H-smooth, then by following the argument in Theorem XIII.24, one can show that $\Gamma_H^+(B^*B) \equiv \text{s-lim}_{s\to\infty}\, i\int_0^s e^{itH}B^*Be^{-itH}\,dt$ exists. Now,

$$\begin{aligned}[H, \Gamma_H^+(B^*B)] &= \operatorname*{s-lim}_{s\to\infty} i\int_0^s e^{itH}[H, B^*B]e^{-itH}\,dt \\ &= \operatorname*{s-lim}_{s\to\infty} (e^{isH}B^*Be^{-isH} - B^*B) \\ &= -B^*B\end{aligned}$$

where we have used the fact that $e^{itH}B^*Be^{-itH}\varphi \in L^2$ with a uniformly bounded derivative to conclude that $\text{s-lim}_{s\to\infty}(e^{isH}B^*Be^{-isH}) = 0$ (Problem 62). Letting $A = i\Gamma_H^+(B^*B)$, we see that $i[H, A] = B^*B$.

We want to apply the idea of positive commutators to prove that N-body Schrödinger operators with repulsive potentials have purely absolutely continuous spectrum. A repulsive potential is a function on $\mathbb{R}^m$ so that $V(r\hat{e}) \le V(r'\hat{e})$ for each unit vector $\hat{e}$ and all $r > r'$. Thus repulsive potentials tend to push particles apart, so we expect no bound states and thus only absolutely continuous spectra. There is another way of describing the fact that V is repulsive that makes the connection with positive commutators clearer. Let $U(\theta)$ be the family of dilations, $(U(\theta)\psi)(r) = e^{+m\theta/2}\psi(e^\theta r)$. Then $[U(\theta)VU(\theta)^{-1}](r) = V(e^\theta r)$, so repulsive potentials obey the condition that $V_\theta \equiv U(\theta)VU(\theta)^{-1}$ is monotone decreasing as θ increases. Since $U(\theta)H_0U(\theta)^{-1} = e^{-2\theta}H_0$, the kinetic energy also decreases monotonically under dilations. Thus, formally,

$$\frac{d}{d\theta}U(\theta)(H_0 + V)U(\theta)^{-1} \leq 0$$

Letting

$$D = \frac{i}{2}\sum_{i=1}^{m}\left(x_i\frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}x_i\right)$$

be the generator of $U(\theta)$ (i.e., $U(\theta) = \exp(-i\theta D)$), we see that $i[D, H] \geq 0$ formally.

Physically, there is another way of looking at the fact that $i[D, H] \geq 0$. For $D = -(i/2)[H, x^2]$. Therefore, if one defines the Heisenberg picture moment of inertia

$$I(t) = e^{+iHt}x^2e^{-iHt}$$

then on a formal level $i[D, H] \geq 0$ is equivalent to $\ddot{I}(t) \geq 0$. It is easy to see that classically the repulsive potential obeys this condition and indeed we have used similar ideas in Theorem XI.3.

Theorem XIII.28 is not directly applicable for three reasons: (1) The computations were formal; as usual this requires care with domains and cores, but it turns out that no extra technical assumption is needed. (2) H is not bounded. It turns out that since H is positive, this in itself would not be very serious (see Problem 61). (3) D is not bounded. This is more serious. The d/dx piece of D is not hard to control since it is H-bounded but the factor of x is hard to control directly. In the proof of the theorem below, we will use a cutoff x which will have the effect of making the computations more complicated. Since V being repulsive is related to $dV/dr \leq 0$, it is the derivative in D rather than the x that is important—thus cutting off x will not destroy $i[A, H] \geq 0$.

Theorem XIII.29 (Lavine's theorem) Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^m)$ ($m \geq 3$). Let V be a function on $\mathbb{R}^m$ so that

(i) Multiplication by V is H_0-bounded with relative bound zero.
(ii) The distributional derivative $\sum_{i=1}^{n} x_i\,\partial V/\partial x_i$ is negative.

Then $H = H_0 + V$ has purely absolutely continuous spectrum.

Proof Choose α obeying $\frac{1}{2} < \alpha < \frac{3}{2}$ and define $g(r) = \int_0^r (1 + \rho^2)^{-\alpha}\, d\rho$. Let A be the operator

$$Af = i \sum_{k=1}^{m} \left[x_k \frac{g(r)}{r} \frac{\partial f}{\partial x_k} + \frac{\partial}{\partial x_k}\left(x_k \frac{g(r) f}{r} \right) \right] \tag{45}$$

Since $g(r)r^{-1}$ is C^∞, A maps C_0^∞ into itself. If g were replaced by r in (45), the operator resulting would be the generator of dilations, so (45) is a partially cutoff version of this generator. In fact, A has a direct geometrical interpretation. Let $T_\gamma\colon \mathbb{R}^n \to \mathbb{R}^n$ be defined by the conditions: $T_0(x) = x$, and $y(\gamma) = T_\gamma x$ solves $\dot{y} = |y|^{-1} g(|y|) y$. Then,

$$(e^{-i\gamma A} f)(x) = N_\gamma(x) f(T_\gamma x)$$

where $N_\gamma(x)$ is a normalizing factor (the square root of a Jacobian determinant).

Our first goal is to prove that for some constant $c > 0$,

$$i[A, H] \geq c(1 + r^2)^{-\alpha - 1}$$

in the sense that for all $\varphi \in C_0^\infty(\mathbb{R}^n)$,

$$i(A\varphi, H\varphi) - i(H\varphi, A\varphi) \geq c(\varphi, (1 + r^2)^{-\alpha - 1}\varphi) \tag{46}$$

First, we compute

$$\begin{aligned} &i(A\varphi, V\varphi) - i(V\varphi, A\varphi) \\ &\quad = 2 \operatorname{Re} \sum_{i=1}^{m} \int V(x) \left[\overline{\varphi(x)} \left\{ \frac{x_i}{r} g(r) \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\frac{x_i}{r} g(r) \right) \right\} \varphi(x) \right] dx \\ &\quad = 2 \int V(x) \sum_{i=1}^{m} \frac{\partial}{\partial x_i} x_i \left(\frac{g(r)}{r} |\varphi(x)|^2 \right) dx \geq 0 \end{aligned}$$

by hypothesis (ii). Thus we need only verify (46) when $V = 0$, a tedious but not too difficult task. As a preliminary, we note that for all r,

$$rg'(r) - g(r) \leq 0 \tag{47a}$$

$$g''(r) = -2\alpha r(1 + r^2)^{-\alpha - 1} \tag{47b}$$

$$g'''(r) + (2\alpha + 1)r^{-1} g''(r) \leq 0 \tag{47c}$$

To prove (47a), we remark that $(1 + r^2)^{-\alpha}$ is monotone decreasing, so its average value $g(r)r^{-1} = r^{-1} \int_0^r (1 + \rho^2)^{-\alpha}\, d\rho$ is also monotone decreasing. Since $rg' - g = r^2(r^{-1}g)'$, (47a) is proven. (47b) and (47c) follow from the explicit calculations:

$$g''(r) = -2\alpha r(1 + r^2)^{-\alpha - 1}$$

$$g'''(r) + (2\alpha + 1)r^{-1} g''(r) = -4\alpha(\alpha + 1)(1 + r^2)^{-\alpha - 2}$$

Next we prove that

$$-\Delta\left(\sum_{j=1}^{m}\frac{\partial g_j}{\partial x_j}\right)\geq c(1+r^2)^{-\alpha-1} \tag{48}$$

where $g_j(x)=x_j r^{-1}g(r)$. For

$$\frac{\partial g_j}{\partial x_k}=r^{-1}g(\delta_{jk}-r^{-2}x_j x_k)+r^{-2}x_j x_k g' \tag{49}$$

Thus

$$\sum_{j=1}^{m}\frac{\partial g_j}{\partial x_j}=(n-1)r^{-1}g+g'$$

Using the fact that for a spherically symmetric function h,

$$\Delta h=r^{-1}(rh)''+(n-3)r^{-1}h'$$

we find that

$$\begin{aligned}-\Delta\left(\sum_{j=1}^{n}\frac{\partial g_j}{\partial x_j}\right)&=-(g'''+(2\alpha+1)r^{-1}g'')-(2n-2\alpha-3)r^{-1}g''\\&\quad-(n-1)(n-3)r^{-3}(rg'-g)\end{aligned}$$

Since $n\geq 3$ and $\alpha<\frac{3}{2}$, (48) follows from (47). Finally, we compute on C_0^{∞} functions that

$$\begin{aligned}-\left[g_k\frac{\partial}{\partial x_k},H_0\right]&=\sum_{i=1}^{n}\left[g_k\frac{\partial}{\partial x_k},\frac{\partial^2}{\partial x_i^2}\right]\\&=\sum_{i=1}^{n}2p_i\frac{\partial g_k}{\partial x_i}p_k+i\frac{\partial^2 g_k}{\partial x_i^2}p_k\end{aligned}$$

where $p_k=i^{-1}\,\partial/\partial x_k$. Using

$$-\left[g_k\frac{\partial}{\partial x_k}+\frac{\partial}{\partial x_k}g_k,H_0\right]=-\left[g_k\frac{\partial}{\partial x_k},H_0\right]-\left[g_k\frac{\partial}{\partial x_k},H_0\right]^*$$

we see that

$$i[A,H_0]=\sum_{i,k}2p_k\left(\frac{\partial g_i}{\partial x_k}+\frac{\partial g_k}{\partial x_i}\right)p_i-\Delta\left(\sum_j\frac{\partial g_j}{\partial x_j}\right)$$

Thus by (48) the proof of (46) has been reduced to proving

$$\sum_{i,}2p_k\left(\frac{\partial g_i}{\partial x}+\frac{\partial g_k}{\partial x_i}\right)p_i\geq 0 \tag{50}$$

By (49) the left-hand side of (50) is

$$4 \sum_{i,k} \{p_k[(r^{-1}g)(\delta_{ik} - r^{-2}x_i x_k)]p_i + p_k(r^{-2}g')x_i x_k p_i\}$$

Fix $x \in \mathbb{R}^n$. Then, by the Schwarz inequality, the matrix $\{\delta_{ik} - r^{-2}x_i x_k\}$ is positive definite. Further, $\{x_i x_k r^{-2}\}$ is clearly positive definite, so (50) holds and this completes the proof of (46).

Next, we need to know that $A < < H$, i.e., that A is H-bounded with relative bound zero. Since $V < < H_0$ by hypothesis, we need only prove that $A < < H_0$. But $\partial/\partial x_i < < H_0$, $x_i g r^{-1}$ is bounded, and

$$A = 2i \sum_{i=1}^{n} x_i g r^{-1}\, \partial/\partial x_i + i(n-1)r^{-1}g + ig'$$

so $A < < H_0$ is proven. Since C_0^∞ is a core for H and $A < < H$, (46) holds for all $\varphi \in D(H)$.

Now let $\varphi \in D(H)$ and let B be multiplication by $c^{1/2}(1+r^2)^{-(\alpha+1)/2}$. Then we claim that

$$\int_{-\infty}^{\infty} \|Be^{-itH}\varphi\|^2\, dt \le d\|(H+I)\varphi\|^2 \tag{51}$$

for a suitable constant d. For, by (46),

$$\begin{aligned}
&\int_{-\infty}^{\infty} \|Be^{-itH}\varphi\|^2\, dt \\
&\quad= \int_{-\infty}^{\infty} (e^{-itH}\varphi, B^*Be^{-itH}\varphi)\, dt \\
&\quad\le \int_{-\infty}^{\infty} i\{(Ae^{-itH}\varphi, He^{-itH}\varphi) - (He^{-itH}\varphi, Ae^{-itH}\varphi)\}\, dt \\
&\quad\le 2 \sup_{-\infty<s<\infty} |(e^{-isH}\varphi, Ae^{-isH}\varphi)|, \\
&\quad\le 2\|\varphi\|\, \|A(H+I)^{-1}\|\, \|(H+I)\varphi\|
\end{aligned}$$

which proves (51).

To conclude the proof we notice that (51) implies that $B(H+I)^{-1}$ is H-smooth. Since $\operatorname{Ran}(B^*)$ and $\operatorname{Ran}(H+I)^{-1}$ are dense, the closure of $\operatorname{Ran}(H+I)^{-1}B^*$ is $\mathscr{H}$. Theorem XIII.23 thus implies that $\mathscr{H} \subset \mathscr{H}_{\mathrm{ac}}$. Therefore H has purely absolutely continuous spectrum. ∎

Corollary Let $m(N-1) \geq 3$. Let $\tilde{H}_0 = \sum_{i=1}^N (-2\mu_i)^{-1} \Delta_i$ on $L^2(\mathbb{R}^{Nm})$ and let H_0 be $\tilde{H}_0$ with its center of mass motion removed. For each i, j suppose that $V_{ij}\colon \mathbb{R}^m \to \mathbb{R}$ and

(i) $V_{ij} \in L^p(\mathbb{R}^m) + L^\infty(\mathbb{R}^m)$ ($p = 2$ if $m \leq 3$, $p > 2$ if $m = 4$; $p = m/2$ if $m \geq 5$).
(ii) $\sum_{k=1}^m x_k\, \partial V_{ij}/\partial x_k \leq 0$ in the distributional sense.

Then the operator $H = H_0 + \sum_{i<j} V_{ij}(r_i - r_j)$ on $L^2(\mathbb{R}^{m(N-1)})$ has purely absolutely continuous spectrum.

Proof Let ζ be a Jacobi coordinate system so $H_0 = \sum_{i=1}^{N-1} (-2M_i)^{-1} \Delta_{\zeta_i}$ and let $q_i = (2M_i)^{1/2}\zeta_i$ so $H_0 = -\sum_{i=1}^{N-1} \Delta_{q_i}$. If we can show that $\sum_{i=1}^{N-1} q_i \cdot \nabla_{q_i} V_{jk} \leq 0$ for all j, k, then the result follows from Theorem XIII.29. Suppose first that each V_{jk} is smooth. Then $V_{jk} = V_{jk}(\sum_{i=1}^{N-1} \alpha_i q_i)$ for suitable α_i. So

$$\sum_i q_i \cdot \nabla_{q_i} V_{jk}\Big(\sum_\ell \alpha_\ell q_\ell\Big) = \Big(\sum_i \alpha_i q_i\Big) \cdot (\nabla_r V_{jk})(r)\Big|_{r=\sum \alpha_\ell q_\ell} = (r \cdot \nabla_r V_{jk})(r)\Big|_{r=\sum \alpha_\ell q_\ell}$$

This is nonpositive by hypothesis. For arbitrary V_{jk}, we average with test functions and mimic the above argument. ∎

C. Local smoothness and wave operators for repulsive potentials

As a final topic in the theory of smooth operators, we shall discuss an extension of Theorem XIII.24. The "trouble" with that theorem is that its conclusion is too strong—H and H_0 are unitarily equivalent. In particular, the theorem cannot be applied to quantum Hamiltonians that have any pure point spectrum. We thus introduce a weaker notion than smoothness.

Definition Let H be a self-adjoint operator with spectral projections E_Ω. We say that A is **H-smooth on Ω**, a Borel set, if and only if AE_Ω is H-smooth.

Theorem XIII.30 Let H be self-adjoint with resolvent R and spectral projections $\{E_\Omega\}$. Let $\Omega \subset \mathbb{R}$. Suppose that $D(A) \supset D(H)$ and that *either*

(a) $\sup_{0<|\varepsilon|<1,\, \lambda\in\Omega} |\varepsilon|\, \|AR(\lambda + i\varepsilon)\|^2 < \infty$

or

(b) $\sup_{0<\varepsilon<1,\, \lambda\in\Omega} \|AR(\lambda + i\varepsilon)A^*\| < \infty$

Then A is H-smooth on $\bar{\Omega}$, the closure of Ω.

Proof (a) For each $\varepsilon \neq 0$, $\|AR(\lambda + i\varepsilon)\|$ is continuous in λ, so the bound

$$C = \sup\{|\varepsilon| \, \|AR(\lambda + i\varepsilon)\|^2 \mid \lambda \in \Omega, 0 < |\varepsilon| < 1\}$$

extends to all $\lambda \in \bar{\Omega}$. Suppose $\lambda \in \mathbb{R}\backslash\bar{\Omega}$. Choose $\lambda_0 \in \bar{\Omega}$ with $|\lambda - \lambda_0| = \text{dist}(\lambda, \bar{\Omega})$. Then

$$\begin{aligned}
&|\varepsilon| \, \|AR(\lambda + i\varepsilon)E_{\bar{\Omega}}\varphi\|^2 \\
&\qquad = |\varepsilon| \, \|AR(\lambda_0 + i\varepsilon)[I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon)]E_{\bar{\Omega}}\varphi\|^2 \\
&\qquad \leq |\varepsilon| \, \|AR(\lambda_0 + i\varepsilon)\|^2 \|(I - (\lambda_0 - \lambda)R(\lambda + i\varepsilon))E_{\bar{\Omega}}\|^2 \|\varphi\|^2 \\
&\qquad \leq 4|\varepsilon| \, \|AR(\lambda_0 + i\varepsilon)\|^2 \|\varphi\|^2
\end{aligned}$$

since $|\lambda_0 - \lambda| \, |x - \lambda + i\varepsilon|^{-1} < 1$ for any $x \in \bar{\Omega}$. Thus

$$\sup_{\substack{\lambda \in \mathbb{R} \\ \varepsilon \neq 0}} |\varepsilon| \, \|AR(\lambda + i\varepsilon)E_{\bar{\Omega}}\| < \infty$$

so $AE_{\bar{\Omega}}$ is H-smooth by Theorem XIII.25 and the remark following its statement.

(b) Since $(AR(\lambda + i\varepsilon)A^*)^* = AR(\lambda - i\varepsilon)A^*$,

$$c = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \|AR(\lambda + i\varepsilon)A^*\| < \infty$$

Thus

$$\begin{aligned}
&\sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \, \|R(\lambda + i\varepsilon)A^*\|^2 \\
&\qquad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} |\varepsilon| \, \|AR(\lambda + i\varepsilon)R(\lambda - i\varepsilon)A^*\| \\
&\qquad = \sup_{\substack{\lambda \in \Omega \\ 0 < |\varepsilon| < 1}} \tfrac{1}{2}\|A[R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)]A^*\| \leq c < \infty
\end{aligned}$$

Since $\|R(\lambda + i\varepsilon)A^*\| = \|AR(\lambda - i\varepsilon)\|$, the conditions of (a) hold. ∎

We can now state the extension of Theorem XIII.24.

Theorem XIII.31 Let H and H_0 be self-adjoint operators with spectral projections E_Ω and $E_\Omega^{(0)}$. Suppose that

$$H - H_0 = A^*B$$

in the sense of (35). Suppose that A is H-bounded and H-smooth on some bounded open interval $\Omega \subset \mathbb{R}$ and that B is H_0-bounded and H_0-smooth on Ω. Then the limits

$$W_\pm = \underset{t \to \mp \infty}{\text{s-lim}}\, e^{iHt} e^{-iH_0 t} E_\Omega^{(0)}$$

and

$$\tilde{W}_\pm = \underset{t \to \mp \infty}{\text{s-lim}}\, e^{iH_0 t} e^{-iHt} E_\Omega$$

exist. Moreover,

$$W_\pm^* = \tilde{W}_\pm \tag{52}$$

$$\tilde{W}_\pm W_\pm = E_\Omega^{(0)}; \qquad W_\pm \tilde{W}_\pm = E_\Omega \tag{53}$$

Proof Suppose that we prove that $W_\pm$ exist and that $\operatorname{Ran} W_\pm \subset E_\Omega$. Then, by symmetry, and the fact that $H_0 - H = -B^*A$, $\tilde{W}_\pm$ exist and $\operatorname{Ran} \tilde{W}_\pm \subset E_\Omega^{(0)}$. (52) is obvious, and (53) follows from the fact that $W_\pm$ (respectively $W_\pm$) is a partial isometry with initial space $E_\Omega^{(0)}$ (respectively E_Ω). We shall show that $W_\pm$ exist and $\operatorname{Ran} W_\pm \subset E_\Omega$ by proving that $\text{s-lim}_{t \to \mp\infty} E_\Omega e^{iHt} e^{-iH_0 t} E_\Omega^{(0)}$ exists and

$$\underset{t \to \mp \infty}{\text{s-lim}}\, E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} E_\Omega^{(0)} = 0 \tag{54}$$

The proof that the first limit exists is identical to the proof of Theorem XIII.24. It is obviously sufficient to prove (54) with $E_\Omega^{(0)}$ replaced by $E_I^{(0)}$ for an arbitrary compact subinterval $I \subset \Omega$. Given such an I, let C be the contour in Figure XIII.4. Then

$$\begin{aligned} & E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} E_I^{(0)} \varphi \\ &= \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} (H - z)^{-1} e^{iHt} e^{-iH_0 t} E_I^{(0)} \varphi \, dz \\ &\quad - \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} e^{iHt} e^{-iH_0 t} (H_0 - z)^{-1} E_I^{(0)} \varphi \, dz \\ &= \frac{1}{2\pi i} \oint_C E_{\mathbb{R}\setminus\Omega} e^{iHt} [(H - z)^{-1} - (H_0 - z)^{-1}] e^{-iH_0 t} E_I^{(0)} \varphi \, dz \end{aligned}$$

Since this last integrand is uniformly bounded on C, it is sufficient, by the dominated convergence theorem, to prove that

$$\underset{t \to \mp \infty}{\text{s-lim}} [(H - z)^{-1} - (H_0 - z)^{-1}] e^{-iH_0 t} E_I^{(0)} = 0 \tag{55}$$

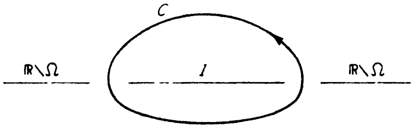


FIGURE XIII.4 A contour of integration.

for all nonreal z. But

$$\begin{aligned}
&|(\psi, [(H-z)^{-1} - (H_0 - z)^{-1}]e^{-iH_0 t}E_I^{(0)}\varphi)| \\
&\quad = |(A(H-z)^{-1}\psi, B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi)| \\
&\quad \le \|A(H-z)^{-1}\| \, \|B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi\| \, \|\psi\|
\end{aligned}$$

Thus, to prove (55) we need only show

$$\lim_{t \to \pm\infty} \|B(H_0 - z)^{-1}e^{-iH_0 t}E_I^{(0)}\varphi\| = 0 \tag{56}$$

But, by the smoothness hypothesis, the function of t in (56) is square-integrable. Moreover, it has a uniformly bounded derivative, so (56) holds (Problem 62). ▌

Corollary Suppose that H and H_0 are self-adjoint with spectral projections E_Ω and $E_\Omega^{(0)}$ and that

$$H - H_0 = A^*B$$

where B is H_0-bounded and A is H-bounded. Let $S \subset \mathbb{R}$ with $S = \bigcup_{i=1}^\infty \Omega_i$ and each Ω_i a bounded open interval. Suppose that:

(i) A is H-smooth on each Ω_i and B is H_0-smooth on each Ω_i.
(ii) Both $\sigma(H)\backslash S$ and $\sigma(H_0)\backslash S$ have Lebesgue measure zero.

Then the generalized wave operators s-$\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0 t}E_{\text{ac}}^{(0)}$ exist and are complete.

Proof Since $S = \bigcup_{i=1}^\infty \Omega_i$ and $E_{\text{ac}}^{(0)} = E_S^{(0)}$, existence follows if we can prove that $\lim_{t\to\mp\infty} e^{iHt}e^{-iH_0 t}\varphi$ exists for $\varphi \in \bigcup_{i=1}^\infty \operatorname{Ran} E_{\Omega_i}^{(0)}$. This is a direct consequence of the theorem. Since the inverse wave operators exist by symmetry, the wave operators are complete. ▌

One application of this corollary will be given in Section 8. Here we apply it to prove a result in the theory of repulsive potentials. This result is not the best possible (see the Notes).

Theorem XIII.32 Let H be an operator of the form given in the corollary of Theorem XIII.29. Suppose that each V_{ij} is a function of $|x|$ obeying $|V_{ij}(x)| \leq C(1 + |x|)^{-\frac{5}{2}-\varepsilon}$ for each i and j and some $\varepsilon > 0$. Then the wave operators $\Omega^{\pm} = \text{s-lim}_{t\to\mp\infty} e^{iHt}e^{-iH_0t}$ exist and are unitary.

Proof Since we already know that H has purely absolutely continuous spectrum, it is sufficient to prove that the wave operators exist and are complete. In the notation used in the proof of Theorem XIII.29, let

$$A_{jk} = +i\left[g(r_j - r_k)\frac{d}{dr_{jk}} + \frac{d}{dr_{jk}}g(r_j - r_k)\right], \qquad A = \sum_{j=k} A_{jk}$$

where $r_{jk} = |r_j - r_k|$ and d/dr_{jk} is defined by

$$r_{jk}\frac{d}{dr_{jk}} = (r_j - r_k)\cdot(\nabla_j - \nabla_k)$$

Now, $i[A_{ij}, V_{ij}] \geq 0$ as in the proof of Theorem XIII.29 and $i[A_{kl}, V_{ij}] = 0$ for i, j, k, l distinct. Finally, for i, j, k distinct,

$$i[A_{ik} + A_{kj}, V_{ij}(r_{ij})] = \mathbf{a}(i, j, k)\cdot(\nabla V_{ij})(r_{ij})$$

where $\mathbf{a}(i, j, k) = g(r_{ik})\mathbf{e}_{ik} + g(r_{kj})\mathbf{e}_{kj}$ and $\mathbf{e}_{ik} = r_{ik}^{-1}(\mathbf{r}_i - \mathbf{r}_k)$. Since V_{ij} is only a function of $|x|$ and $(\mathbf{x}\cdot\nabla)V_{ij} \leq 0$, we can conclude that $i[A_{ik} + A_{kj}, V_{ij}] \geq 0$ if $(\mathbf{r}_i - \mathbf{r}_j)\cdot(\mathbf{a}(i, j, k)) \geq 0$. But

$$\begin{aligned}(\mathbf{r}_i - \mathbf{r}_j)\cdot\mathbf{a}(i, j, k) &= r_{ik}g(r_{ik}) + r_{kj}g(r_{kj})\\ &\quad + (e_{ik}\cdot e_{kj})(r_{ik}g(r_{kj}) + r_{kj}g(r_{ik}))\\ &\geq (r_{ik} - r_{kj})(g(r_{ik}) - g(r_{jk}))\\ &\geq 0\end{aligned}$$

since g is monotone. It follows that $i[A, V] \geq 0$ so that computations identical to those used in Theorem XIII.29 show that (Problem 64):

$$i[A, H] \geq c(1 + r_{jk})^{-3-\varepsilon}$$

for a suitable constant c. Again, following the proof of Theorem XIII.29, we conclude that $(1 + r_{jk})^{-\frac{3}{2}-\varepsilon}(H + I)^{-1}$ is H-smooth. Since

$$\|\,|V_{ij}|^{3/5}(H + I)^{-1}e^{-iHt}\varphi\| \leq c^{1/2}\|(1 + r_{jk})^{-\frac{3}{2}-\varepsilon}(H + I)^{-1}e^{-iHt}\varphi\|$$

$|V_{ij}|^{3/5}(H + I)^{-1}$ is H-smooth and thus $|V_{ij}|^{3/5}$ is H-smooth on any compact set. By hypothesis, $|V_{ij}|^{2/5} \in L^{m+\varepsilon}(\mathbb{R}^m) \cap L^{m-\varepsilon}(\mathbb{R}^m)$, so by the proof of Theorem XIII.27, $|V_{ij}|^{2/5}$ is H_0-smooth. The result now follows from the previous corollary. ∎

XIII.8 The absence of singular continuous spectrum III: Weighted L^2 spaces

We have seen that a sufficient condition for $\sigma_{\text{sing}}(H)$ to be empty is that there be a dense set of vectors $X \subset \mathscr{H}$ so that $(\varphi, (H-z)^{-1}\varphi)$ remains bounded as $z \to \lambda \in \mathbb{R}$ for any $\varphi \in X$. There is a natural way of approaching this condition. Suppose that $X \subset \mathscr{H}$ is dense and that there is a norm $|||\cdot|||_+$ on X so that X is a Banach space and so that $|||\varphi|||_+ \geq \|\varphi\|$ for any $\varphi \in X$. Then the inner product on $\mathscr{H}$ allows one to realize $\mathscr{H}$ in a natural way as a subset of X^*. If $|||\cdot|||_-$ denotes the norm on X^*, then $\|\varphi\| \geq |||\varphi|||_-$ for any $\varphi \in \mathscr{H}$. We have already discussed such a situation and related ideas in Section VIII.6 and the appendix to Section XI.6. Let $z \in \mathbb{C}$ with $\operatorname{Im} z \neq 0$. Then $(H-z)^{-1}$ takes $\mathscr{H}$ into $\mathscr{H}$ and so X into X^*. Of course the norm of $(H-z)^{-1}$ as a map from $\mathscr{H}$ to $\mathscr{H}$ diverges as z approaches $\sigma(H)$, but suppose that it remains bounded as a map of X into X^*. Then

$$|(\varphi, (H-z)^{-1}\varphi)| \leq |||\varphi|||_+^2 \, \|(H-z)^{-1}\|_{+,-}$$

where

$$\|A\|_{+,-} = \sup_{\psi \neq 0,\, \psi \in X} \|A\psi\|_- / \|\psi\|_+$$

so we can conclude that $\sigma_{\text{sing}}(H) = \varnothing$, by Theorem XIII.20.

It is natural to try to implement this idea with perturbation techniques. That is, we consider $H = H_0 + V$ and begin by proving bounds on $(H_0 - z)^{-1}$ as a map from X to X^*. We shall consider Schrödinger operators and take $H_0 = -\Delta$. To motivate our choice of X, let $f \in \mathscr{S}(\mathbb{R}^n)$ and consider

$$\begin{aligned}\lim_{y \downarrow 0} & (f, [(H_0 - x + iy)^{-1} - (H_0 - x - iy)^{-1}]f) \\ &= \lim_{y \downarrow 0} \int |\hat{f}(p)|^2 2i \operatorname{Im}[(p^2 - x + iy)^{-1}]\, d^n p \\ &= -2i\pi \int |\hat{f}(p)|^2 \, \delta(p^2 - x)\, d^n p\end{aligned}$$

by Eq. (V.4). Thus, for $(f, (H_0 - x + iy)^{-1} f)$ to have a limit as $y \downarrow 0$, $\hat{f}$ must have a "natural" restriction to the sphere of radius $x^{1/2}$. Because of our discussion in Section IX.9, it is natural to choose X as an L_δ^2 space (with $\delta > \frac{1}{2}$) so that X^* is $L_{-\delta}^2$:

$$L_\delta^2(\mathbb{R}^n) = \left\{ f(x) \,\middle|\, \|f\|_\delta^2 \equiv \int (1 + x^2)^\delta |f(x)|^2 \, dx < \infty \right\}$$

We shall lean heavily on the estimates proven in Section IX.9, especially Theorems IX.39 and IX.41.

Definition A multiplication operator is called an **Agmon potential** if $V(x) = (1 + x^2)^{-\frac{1}{2}-\varepsilon}W(x)$ for some $\varepsilon > 0$ and some W that is a relatively compact perturbation of $-\Delta$.

The Agmon potentials form a vector space of $-\Delta$-bounded perturbations of relative bound zero (see Problem 20 of Chapter X).

Example 1 Let $p > n/2$, $p < \infty$, and $p \geq 2$. Then any $W \in L^p(\mathbb{R}^n)$ is relatively compact (Problem 41), so any V with $(1 + x^2)^{\frac{1}{2}+\varepsilon}V \in L^p$ is an Agmon potential.

Example 2 Let $W \in L^\infty(\mathbb{R}^n)$ and define $V(x) = (1 + x^2)^{-\frac{1}{2}-\varepsilon}W(x)$. To show that V is an Agmon potential we need only prove that $U(x) = (1 + x^2)^{-\varepsilon/2}W(x)$ is relatively compact. But this is true since $U(x)$ is in $L^p + (L^\infty)_\varepsilon$ for all p (Problem 41).

The main theorem of this section is:

Theorem XIII.33 (the Agmon–Kato–Kuroda theorem) Let V be an Agmon potential and let $H = H_0 + V$ where $H_0 = -\Delta$. Then:

(a) The set $\mathscr{E}_+$ of positive eigenvalues of H is a discrete subset of $(0, \infty)$, and each eigenvalue has finite multiplicity.

(b) If C is any compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$ and if $\delta > \frac{1}{2}$, then

$$\sup_{\lambda \in C,\, 0 < y < 1} \quad \sup_{\psi,\, \varphi \in L_\delta^2:\, \|\varphi\|_\delta \leq 1,\, \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty$$

(c) $\sigma_{\text{sing}}(H) = \varnothing$.

(d) The wave operators $\Omega^\pm(H, H_0)$ exist and are complete.

The proof of Theorem XIII.33, while elegant, is rather long so we break it up into a series of lemmas. After proving (a), we develop a few technical estimates that will allow us to prove (c) and (d) from (b); then we prove (b) in case $V = 0$; finally, we use the estimates proven for H_0, Theorem IX.39, Theorem IX.41, and a bootstrap argument to complete the proof. Throughout we let $\rho(x) \equiv (1 + x^2)^{1/2}$. The use of the weighted L^2 spaces and Theorem IX.39 is illustrated in:

Proof of (a) of Theorem XIII.33 Suppose that $\varphi \in D(H)$ and $H\varphi = \lambda\varphi$ with $\lambda > 0$. First, we shall show that $\|\varphi\|_\delta \leq c\|\varphi\|$ for some $\delta > 0$ where c depends only on λ and remains bounded as λ varies through compact subsets of

$(0, \infty)$. Since W is H_0-compact, it is H-bounded so that $\|W\varphi\| \le a\|H\varphi\| + b\|\varphi\| = (a\lambda + b)\|\varphi\|$. As a result $\psi \equiv V\varphi = \rho^{-1-\varepsilon}W\varphi$ is in $L^2_{1+\varepsilon}$. In particular, by Theorem IX.40, $\hat{\psi}$ has restrictions to each sphere S_E, and the restriction is Hölder continuous in E. Since $(H_0 - \lambda)\varphi = -\psi$, $\hat{\varphi} = -(k^2 - \lambda)^{-1}\hat{\psi}$. If $\hat{\psi} \restriction S_{\sqrt{\lambda}}$ were not identically zero, then $\hat{\varphi}$ could not be in L^2, so we conclude that $\psi \restriction S_{\sqrt{\lambda}} = 0$. As a result, Theorem IX.41 is applicable, so

$$\|\varphi\|_{\varepsilon/2} \le c_\lambda \|\psi\|_{1+\varepsilon} = c_\lambda \|W\varphi\| \le d_\lambda \|\varphi\|$$

Let $\eta \equiv \rho^{\varepsilon/2}(-\Delta + 1)\varphi$. Then $H\varphi = \lambda\varphi$ implies that

$$\begin{aligned}\|\eta\| &\le \|\rho^{\varepsilon/2}(\lambda + 1)\varphi\| + \|\rho^{\varepsilon/2}V\varphi\| \\ &\le (\lambda + 1)\|\varphi\|_{\varepsilon/2} + \|W\varphi\| \le c'_\lambda \|\varphi\|\end{aligned}$$

Since $\varphi = (-\Delta + 1)^{-1}\rho^{-\varepsilon}\eta$, we conclude that for any compact subset K in $(0, \infty)$, any solution of $H\varphi = \lambda\varphi$ with $\lambda \in K$ and $\|\varphi\| = 1$ is of the form $\varphi = A\eta$ where: (i) $A = (-\Delta + 1)^{-1}\rho^{-\varepsilon}$ and (ii) $\|\eta\| \le c$, a constant only depending on K. By Problem 41, A is a compact operator, so the set $M = \{\varphi = A\eta \mid \|\eta\| \le c\}$ is compact. If any eigenvalue $\lambda \in K$ were of infinite multiplicity or if there were infinitely many eigenvalues in K, M would contain an infinite orthonormal set. Since M is compact, K contains only finitely many eigenvalues and each is of finite multiplicity. ▮

We note that we shall show that $\mathscr{E}_+ = \varnothing$ under some additional regularity hypotheses on V in Section 13.

Lemma 1 Let F and G be any two real-valued multiplication operators that are H_0-bounded with relative bound zero. Then for any $\mu \in \mathbb{C}\backslash\mathbb{R}$, $(H_0 - \mu)^{-1}$, $(H_0 + G - \mu)^{-1}$, $F(H_0 - \mu)^{-1}$, and $F(H_0 + G - \mu)^{-1}$ are bounded on each L^2_δ. Moreover, if F is also H_0-relatively compact, then $F(H_0 - \mu)^{-1}$ and $F(H_0 + G - \mu)^{-1}$ are compact on each L^2_δ.

Proof We shall prove the lemma for $(H_0 - \mu)^{-1}$ in the case $|\delta| \le 1$. The other cases are similar and are left to the problems (Problem 66). Introduce the symbol ∂_j for the operator $\partial/\partial x_j$ and consider the formal computation

$$\begin{aligned}[(H_0 - \mu)^{-1}, \rho^\delta] &= -(H_0 - \mu)^{-1}[H_0, \rho^\delta](H_0 - \mu)^{-1} \\ &= \sum_{i=1}^{n} \{(H_0 - \mu)^{-1}\,\partial_i\}(\partial_i \rho^\delta)(H_0 - \mu)^{-1} \\ &\quad + (H_0 - \mu)^{-1}(\partial_i \rho^\delta)\{\partial_i (H_0 - \mu)^{-1}\}\end{aligned}$$

Applied to vectors in $\mathscr{S}$, all computations are legitimate. Moreover, if $\delta \leq 1$, $\partial_i(\rho^\delta)$ is bounded. Since $(H_0 - \mu)^{-1}$ and $\partial_i(H_0 - \mu)^{-1}$ are bounded on L^2 we conclude that

$$\|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \leq \text{const}\|\psi\|$$

if ψ is in $\mathscr{S}$ and so for arbitrary ψ in L^2. Suppose $1 \geq \delta > 0$. Then

$$\begin{aligned}\|(H_0 - \mu)^{-1}\psi\|_\delta &= \|\rho^\delta(H_0 - \mu)^{-1}\psi\| \\ &\leq \|(H_0 - \mu)^{-1}\| \, \|\psi\|_\delta + \|[(H_0 - \mu)^{-1}, \rho^\delta]\psi\| \\ &\leq d\|\psi\|_\delta\end{aligned}$$

so $(H_0 - \mu)^{-1}$ is bounded from L_δ^2 to L_δ^2. By duality, $(H_0 - \bar{\mu})^{-1}$ is bounded from $L_{-\delta}^2$ to $L_{-\delta}^2$. ∎

Lemma 2 Let $H = H_0 + V$ as in Theorem XIII.33. Suppose that F is an Agmon potential and that for some compact interval $\Omega \subset \mathbb{R}$, and each $\delta > \frac{1}{2}$,

$$\sup_{x \in \Omega,\, 0 < y < 1} \; \sup_{\psi,\, \varphi \in L_\delta{}^2;\; \|\varphi\|_\delta \leq 1,\; \|\psi\|_\delta \leq 1} |(\psi, (H - \lambda - iy)^{-1}\varphi)| < \infty \tag{57}$$

Then $|F|^{1/2}$ is H-smooth on Ω.

Proof By Theorem XIII.30, we need only prove that

$$\sup_{\substack{\lambda \in \Omega \\ 0 < y < 1}} \| |F|^{1/2}(H - \lambda - iy)^{-1} |F|^{1/2}\| < \infty$$

(57) implies that $(H - \lambda - iy)^{-1}$ is uniformly bounded from L_δ^2 to $L_{-\delta}^2$ for $\lambda + iy \in \Omega \times (0, 1)$. Write $F = \rho^{-1-\varepsilon}G$ where G is H_0-compact and let $\delta = \frac{1}{2} + (\varepsilon/2)$. Then, by Lemma 1, $(H - i)^{-1}|G|^{1/2}$ is bounded from L_δ^2 to L_δ^2 so $|G|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|G|^{1/2}$ is uniformly bounded from L_δ^2 to $L_{-\delta}^2$ for $\lambda + iy \in \Omega \times (0, 1)$. Thus

$$|F|^{1/2}(H - i)^{-1}(H - \lambda - iy)^{-1}(H - i)^{-1}|F|^{1/2}$$

is uniformly bounded from L^2 to L^2 for $\lambda + iy \in \Omega \times (0, 1)$. Writing

$$\begin{aligned}(H - z)^{-1} = (H - i)^{-1} &+ (z - i)(H - i)^{-2} \\ &+ (z - i)^2(H - i)^{-1}(H - z)^{-1}(H - i)^{-1}\end{aligned}$$

and using the fact that $\| |F|^{1/2}(H - i)^{-1} |F|^{1/2}\| < \infty$, we see that

$$\sup_{\lambda + iy \in \Omega \times (0, 1)} \| |F|^{1/2}(H - \lambda - iy)^{-1} |F|^{1/2}\| < \infty. \quad ∎$$

Reduction of Theorem XIII.33 to the proof of (b) We want to show that once we prove (b), then (c) and (d) follow. Suppose that (b) holds, that $\varphi \in L^2_\delta$ for $\delta > \frac{1}{2}$, and that K is a compact subinterval of $(0, \infty)\backslash\mathscr{E}_+$. Then $E_K\varphi \in \mathscr{H}_{\text{ac}}$ by Theorem XIII.20. Thus $K \cap \sigma_{\text{sing}} = \varnothing$. By the second corollary to Theorem XIII.14, $\sigma_{\text{ess}} = [0, \infty)$, so we conclude that $\sigma_{\text{sing}} \cap (-\infty, 0) = \varnothing$. Therefore, $\sigma_{\text{sing}} \subset (\mathscr{E}_+ \cup \{0\})$. $\mathscr{E}_+$ is countable by (a), so $\sigma_{\text{sing}} = \varnothing$. Applying Lemma 2 to the case $V = 0$, we see that $|V|^{1/2}$ is H_0-smooth on Ω for any interval $[a, b]$ with $a > 0$. In addition, $|V|^{1/2}$ is H-smooth on any such Ω with $\Omega \cap \mathscr{E}_+ = \varnothing$. (d) now follows from the corollary of Theorem XIII.31. ▌

The remainder of this section is devoted to proving (b). We first prove the case $V = 0$, which is an estimate quite similar to Theorem IX.41. The proof is also quite similar.

Lemma 3 Let $\varepsilon > 0$. Then there exists a constant c so that for all $\lambda \in \mathbb{C}$ and all $\varphi \in \mathscr{S}(\mathbb{R})$

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \le c\left\|\left(\frac{d}{dx} - \lambda\right)\varphi\right\|_{\frac{1}{2}+\varepsilon} \tag{58}$$

Proof Suppose that $\operatorname{Re}\lambda \le 0$. Let $\psi = (d/dx - \lambda)\varphi$. Then

$$\varphi(x) = \int_{-\infty}^{x} e^{\lambda(x-y)}\psi(y)\,dy$$

Thus

$$\begin{aligned}\|\varphi\|_{L^\infty} \le \|\psi\|_{L^1} &= ((1 + x^2)^{-\frac{1}{4}-\frac{1}{2}\varepsilon}, (1 + x^2)^{\frac{1}{4}+\frac{1}{2}\varepsilon}\psi) \\ &\le c_1\|\psi\|_{\frac{1}{2}+\varepsilon}\end{aligned}$$

Since

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \le \|\varphi\|_{L^\infty}\,\|(1 + x^2)^{-\frac{1}{4}-\frac{1}{2}\varepsilon}\|_{L^2}$$

(58) follows in the case $\operatorname{Re}\lambda \le 0$. A similar argument works for $\operatorname{Re}\lambda \ge 0$. ▌

Lemma 4 Let n be fixed. Then for all $\varepsilon > 0$, there is a constant d so that for all $\lambda \in \mathbb{C}$, each $j = 1, \ldots, n$, and all $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\partial_j\varphi\|_{-\frac{1}{2}-\varepsilon} \le d\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{59}$$

Proof Consider first the case $n = 1$. Let $\lambda = -\mu^2$. Then by Lemma 3,

$$\left\| \frac{d}{dx}\varphi \right\|_{-\frac{1}{2}-\varepsilon} \leq \frac{1}{2}\left\| \left(\frac{d}{dx} - \mu\right)\varphi \right\|_{-\frac{1}{2}-\varepsilon} + \frac{1}{2}\left\| \left(\frac{d}{dx} + \mu\right)\varphi \right\|_{-\frac{1}{2}-\varepsilon}$$

$$\leq c\left\| \left(-\frac{d^2}{dx^2} - \lambda\right)\varphi \right\|_{\frac{1}{2}+\varepsilon}$$

Now let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and let $\psi(x_1, k_2, \ldots, k_n)$ be the partial Fourier transform of φ with respect to $x_2, \ldots, x_n$,

$$\psi(x_1, k_2, \ldots, k_n) = (2\pi)^{-(n-1)/2} \int e^{-i\sum_2^n k_j x_j}\varphi(x_1, \ldots, x_n)\, dx_2 \cdots dx_n$$

Using the one-dimensional result, for each fixed $k_2, \ldots, k_n$,

$$\int (1 + x_1^2)^{-\frac{1}{2}-\varepsilon} |\partial_1 \psi(x_1, k_2, \ldots, k_n)|^2\, dx_1$$

$$\leq c \int (1 + x_1^2)^{\frac{1}{2}+\varepsilon} |(-\partial_1^2 + k_2^2 + \cdots + k_n^2 - \lambda)\psi|^2\, dx_1$$

Integrating with respect to $k_2, \ldots, k_n$ and using the Plancherel theorem, we see that

$$\int (1 + x_1^2)^{-\frac{1}{2}-\varepsilon} |\partial_1 \varphi(x)|^2\, d^n x \leq c \int (1 + x_1^2)^{\frac{1}{2}+\varepsilon} |(-\Delta - \lambda)\varphi|^2\, d^n x$$

Since $(1 + x^2)^{-\frac{1}{2}-\varepsilon} \leq (1 + x_1^2)^{-\frac{1}{2}-\varepsilon}$ and $(1 + x_1^2)^{\frac{1}{2}+\varepsilon} \leq (1 + x^2)^{\frac{1}{2}+\varepsilon}$, (59) follows. ▮

Lemma 5 Let n be fixed. For any compact set $K \subset \mathbb{C}\backslash\{0\}$, there is a constant c so that for all $\lambda \in K$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\|\varphi\|_{-\frac{1}{2}-\varepsilon} \leq c\|(-\Delta - \lambda)\varphi\|_{\frac{1}{2}+\varepsilon} \tag{60}$$

Proof We can find $c_1 > 0$ satisfying

$$\inf_{x \in \mathbb{R},\, \lambda \in K} [|x^2 - \lambda|^2 + |x|^2] \geq c_1^{-2}$$

Therefore, given $\psi \in \mathscr{S}(\mathbb{R}^n)$

$$|\hat{\psi}(k_1, \ldots, k_n)|^2 \leq c_1^2 \left[|(\textstyle\sum k_i^2 - \lambda)\hat{\psi}(k_1, \ldots, k_n)|^2 + \displaystyle\sum_{i=1}^n |k_i \hat{\psi}(k_1, \ldots, k_n)|^2 \right]$$

Integrating and using the Plancherel theorem

$$\|\psi\|^2 \leq c_1^2 \left[\|(-\Delta - \lambda)\psi\|^2 + \sum_{j=1}^n \|\partial_j \psi\|^2 \right] \tag{61a}$$

for all $\lambda \in K$. Let α be a positive real number which we shall adjust below. Set $\delta = \frac{1}{2} + \varepsilon$ and $\rho_\alpha = (1 + \alpha x^2)^{1/2}$. Finally, let $\varphi = (\rho_\alpha)^\delta \psi$. Then, by (61a)

$$\|\rho_\alpha^{-\delta}\varphi\| \le c_1 \|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| + c_1 \sum_{j=1}^{n} \|\partial_j \rho_\alpha^{-\delta}\varphi\| \tag{61b}$$

Now $\partial_j \rho_\alpha^{-\delta}\varphi = \rho_\alpha^{-\delta}\, \partial_j \psi - \delta\alpha x_j \rho_\alpha^{-\delta-1}\varphi$ so

$$\|\partial_j \rho_\alpha^{-\delta}\varphi\| \le \|\rho_\alpha^{-\delta}\, \partial_j \varphi\| + \alpha^{1/2}\, \delta \|\rho_\alpha^{-\delta}\varphi\|$$

since $|\alpha^{1/2} x_j \rho^{-1}| \le 1$ for all x. Similarly (Problem 67),

$$\begin{aligned} \|(-\Delta - \lambda)\rho_\alpha^{-\delta}\varphi\| \le \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| &+ 2\, \delta\alpha^{1/2} \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\, \partial_j \varphi\| \\ &+ d_{n,\varepsilon}\alpha \|\rho_\alpha^{-\delta}\varphi\| \end{aligned} \tag{62}$$

where $d_{n,\varepsilon}$ is only dependent on ε and n. Pick α so small that $c_1(n\, \delta\alpha^{1/2} + d_{n,\varepsilon}\alpha) < \frac{1}{2}$ and $\alpha < 1$. Then, by (61), for all $\varphi \in \mathscr{S}$ and $\lambda \in K$,

$$\tfrac{1}{2}\|\rho_\alpha^{-\delta}\varphi\| \le c_2 \left| \|\rho_\alpha^{-\delta}(-\Delta - \lambda)\varphi\| + \sum_{j=1}^{n} \|\rho_\alpha^{-\delta}\, \partial_j \varphi\| \right|$$

Since $\rho^{-\delta} \le \rho_\alpha^{-\delta} \le \alpha^{-\delta/2}\rho^{-\delta}$, we have that

$$\|\varphi\|_{-\delta} \le c_3[\|(-\Delta - \lambda)\varphi\|_{-\delta} + \sum_{j} \|\partial_j \varphi\|_{-\delta}]$$

where c_3 is independent of $\lambda \in K$ and $\varphi \in \mathscr{S}$. Since $\|\cdot\|_{-\delta} \le \|\cdot\|_\delta$ and $\|\partial_j \varphi\|_{-\delta} \le c\|(-\Delta - \lambda)\varphi\|_\delta$ by Lemma 4, (60) follows. ▌

If now $\operatorname{Im} \lambda \ne 0$ and $\delta > \frac{1}{2}$, then by Lemma 1, $(H_0 - \lambda)^{-1}$ is a bounded map from L^2_δ to L^2_δ. Lemma 5 assures us that, for $\lambda \in K = [a, b] \times (0, 1]$ $(a > 0)$, we have the basic estimate

$$\|(H_0 - \lambda)^{-1}\varphi\|_{-\delta} \le c\|\varphi\|_\delta \tag{63}$$

Given (63), it is natural to consider the boundary values $\lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ as maps of L^2_δ to $L^2_{-\delta}$. Such boundary values are not strictly necessary for the proof, but they help to make it more conceptual, so we introduce them. As preparation, we need

Lemma 6 Let $\delta > \frac{3}{2}$ and let $0 < a < b$. Then there is a constant c so that for all $\varphi \in L^2_\delta$ and $\lambda = x + iy$ with $x \in [a, b]$ and $y \in (0, 1]$,

$$\|(H_0 - \lambda)^{-2}\varphi\|_{-\delta} \le c\|\varphi\|_\delta$$

Proof Let A be the operator $\sum_{j=1}^{n} x_j \partial_j$. Then $[A, (H_0 - \lambda)] = -2H_0$ so that

$$\begin{aligned}[A, (H_0 - \lambda)^{-1}] &= -(H_0 - \lambda)^{-1}[A, (H_0 - \lambda)](H_0 - \lambda)^{-1} \\ &= 2H_0(H_0 - \lambda)^{-2} \\ &= 2(H_0 - \lambda)^{-1} + 2\lambda(H_0 - \lambda)^{-2}\end{aligned}$$

where all the computations are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R}^n)$. Since $(H_0 - \lambda)^{-1}$ is uniformly bounded from L_δ^2 to $L_{-\delta}^2$, we need only prove that $[A, (H_0 - \lambda)^{-1}]$ is bounded from L_δ^2 to $L_{-\delta}^2$, uniformly for λ satisfying $a \le \operatorname{Re} \lambda \le b$, $0 < \operatorname{Im} \lambda \le 1$. It is thus sufficient to prove that $\rho^{-\delta}(x_j \partial_j) \times (H_0 - \lambda)^{-1}\rho^{-\delta}$ is bounded on L^2 uniformly in λ. Write

$$(H_0 - \lambda)^{-1} = (H_0 + 1)^{-1} + (\lambda + 1)(H_0 + 1)^{-1}(H_0 - \lambda)^{-1}$$

Certainly $(\rho^{-\delta}x_j)[\partial_j(H_0 + 1)^{-1}]\rho^{-\delta}$ is bounded on L^2. Moreover

$$\rho^{-1}x_j[\rho^{-\delta+1}(\partial_j(H_0 + 1)^{-1})\rho^{\delta-1}](\rho^{-\delta+1}(H_0 - \lambda)^{-1}\rho^{-\delta+1})\rho^{-1}$$

is bounded for the first and last factor are trivially bounded, the third is bounded by Lemma 5, and the second is bounded by mimicking the proof of Lemma 1 (Problem 66c). ∎

Lemma 7 Let $\delta > \frac{1}{2}$ and let $x > 0$. Then $(H_0 - x - i0)^{-1} \equiv \lim_{y \downarrow 0} (H_0 - x - iy)^{-1}$ exists in norm as a map from L_δ^2 to $L_{-\delta}^2$. Moreover:

(a) $V(H_0 - x - i0)^{-1}$ is compact as a map of L_δ^2 to L_δ^2 if V is an Agmon potential such that $\rho^{2\delta}V = W$ is relatively H_0-compact.

(b) $\operatorname{Im}(\varphi, (H_0 - x - i0)^{-1}\varphi) = (\pi/2)x^{\frac{1}{2}n-1} \int_{S^{n-1}} |\hat{\varphi}(x^{1/2}\Omega)|^2 \, d\Omega$ where $\hat{\varphi} \restriction S_{x^{1/2}}$ is defined by Theorem IX.39, and $d\Omega$ is the usual surface measure on the sphere.

Proof Let $\delta' = \delta + 1$. Then as operators from $L_{\delta'}^2$ to $L_{-\delta'}^2$,

$$\begin{aligned}&\|(H_0 - \lambda_1)^{-1} - (H_0 - \lambda_2)^{-1}\| \\ &\qquad \le |\lambda_2 - \lambda_1| \sup_{0 \le t \le 1} \|[H_0 - t\lambda_1 - (1 - t)\lambda_2]^{-2}\|\end{aligned}$$

By Lemma 6, we see that $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. Let $\delta'' = \frac{1}{2}(\delta + \frac{1}{2})$. Then by Lemma 5, $(H_0 - x - iy)^{-1}$ is norm bounded as $y \downarrow 0$ as a map from $L_{\delta''}^2$ to $L_{-\delta''}^2$. Since $\delta'' < \delta < \delta'$, we can interpolate between the

δ' and δ'' results (see Example 3 of the appendix to Section IX.4) and conclude that as maps from L^2_δ to $L^2_{-\delta}$, $(H_0 - x - iy)^{-1}$ is norm Cauchy as $y \downarrow 0$. To prove (a) we write

$$W(H_0 - x - i0)^{-1} = W(H_0 + 1)^{-1} + (x + 1)W(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

and so conclude by Lemma 1 that $W(H_0 - x - i0)^{-1}$ is compact as a map from L^2_δ to $L^2_{-\delta}$. Since $\rho^{-2\delta}$ is an isometry from $L^2_{-\delta}$ to L^2_δ, (a) follows. Finally, (b) holds for $\varphi \in \mathscr{S}$ because of (V.4) (see Problem 22 of Chapter V). By Theorem IX.39, it extends to all $\varphi \in L^2_\delta$. ▮

Lemma 8 Let $\delta > \frac{1}{2}$ and let $\varphi \in L^2_\delta$ satisfy $\varphi = -V(H_0 - x - i0)^{-1}\varphi$ where $x > 0$, and V is an Agmon potential so that $\rho^{2\delta}V = W$ is relatively H_0-compact, and where $V(H_0 - x - i0)^{-1}$ is interpreted as the composition of maps $W(H_0 - x - i0)^{-1}$ from L^2_δ to $L^2_{-\delta}$ and $\rho^{-2\delta}$ from $L^2_{-\delta}$ to L^2_δ. Then:

(a) $\psi \equiv (H_0 - x - i0)^{-1}\varphi$ is in L^2.
(b) If $\varphi \neq 0$, then x is an eigenvalue of $H = H_0 + V$ as an operator on L^2.

Proof The argument is very similar to the proof of (a) of Theorem XIII.33. By the formula

$$(H_0 - x - i0)^{-1} = (H_0 + 1)^{-1} + (x + 1)(H_0 + 1)^{-1}(H_0 - x - i0)^{-1}$$

we see that $\psi \in (H_0 + 1)^{-1}[L^2_{-\delta}]$ so that $W\psi \in L^2_{-\delta}$ by Lemma 1. As a result, the integral $\int V(\xi)\,|\psi(\xi)|^2\, d\xi = (\rho^{-\delta}\psi, \rho^{-\delta}W\psi)$ is absolutely convergent and obviously real. But $V\psi = -\varphi$ so we conclude that $(\varphi, (H_0 - x - i0)^{-1}\varphi)$ is real. By Lemma 7, part (b), $\hat{\varphi} \restriction S_{x^{1/2}} \equiv 0$. As a result, Theorem IX.41 is applicable and we have the following "bootstrap" argument: Let $\delta = \frac{1}{2} + \varepsilon$. Since $\varphi \in L^2_\delta$, $\psi \in L^2_{\delta - 1 - \varepsilon}$ by Theorem IX.41. Using Lemma 1 and

$$W\psi = W(H_0 + 1)^{-1}\varphi + (x + 1)W(H_0 + 1)^{-1}\psi$$

we see that $W\psi \in L^2_{\delta - 1 - \varepsilon}$ also. Thus $\varphi = -V\psi = -\rho^{2\delta}W\psi$ is in $L^2_{\delta - 1 - \varepsilon + 2\delta} = L^2_{\delta + \varepsilon}$. By this argument we have improved the estimate $\varphi \in L^2_\delta$ to $\varphi \in L^2_{\delta + \varepsilon}$. There is nothing to stop us from repeating it! Thus, $\varphi \in L^2_{\delta + n\varepsilon}$ for all n so $\psi \in L^2_{\delta - 1 + (n-1)\varepsilon}$ for all n. In particular $\psi \in L^2$. For $\eta \in \mathscr{S}$,

$$\begin{aligned}(H_0\eta, \psi) = \lim_{y \downarrow 0}\, (\eta, H_0(H_0 - x - iy)^{-1}\varphi) &= \lim_{y \downarrow 0}\, (\eta, (x + iy)\psi + \varphi) \\ &= (\eta, x\psi + \varphi)\end{aligned}$$

Therefore, $\psi \in D(H_0)$ and $H_0\psi = x\psi + \varphi = x\psi - V\psi$ so x is an eigenvalue of H as an operator on L^2. ▮

Completion of the proof of Theorem XIII.33 Choose $\delta > \frac{1}{2}$ so that $\rho^{2\delta}V = W$ is relatively H_0-compact. Given a compact subinterval $K \subset (0, \infty)\backslash\mathscr{E}_+$, consider the operator-valued function $A(\mu) = V(H_0 - \mu)^{-1}$ on $K \times [0, 1]$ where $(H_0 - \mu)^{-1}$ is interpreted as $(H_0 - x - i0)^{-1}$ if $\operatorname{Im} \mu = 0$. Then $A(\mu)$ is a function with values in the compact operators on L^2_δ, continuous on $K \times [0, 1]$ and analytic in its interior. Moreover, $A(\mu)\varphi = -\varphi$ has no nonzero solutions for $\mu \in K \times [0, 1]$. When $\operatorname{Im} \mu = 0$, this follows from the hypothesis $K \cap \mathscr{E}_+ = \emptyset$ and Lemma 8. For $\operatorname{Im} \mu \neq 0$, this follows from the facts that $(1 + V(H_0 - \mu)^{-1})(H_0 - \mu) = H - \mu$ and that both $H_0 - \mu$ and $H - \mu$ are invertible as maps of L^2_δ to L^2_δ by Lemma 1. It follows by a simple extension of the analytic Fredholm theorem (Theorem VI.14) that $(1 + A(\mu))^{-1}$ is a continuous function on $K \times [0, 1]$; in particular, it is uniformly bounded. But for $\operatorname{Im} \mu \neq 0$, $(H - \mu)^{-1} = (H_0 - \mu)^{-1} \times (1 + A(\mu))^{-1}$. Since $(H_0 - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ by Lemma 5 and $(1 + A(\mu))^{-1}$ is uniformly bounded from L^2_δ to L^2_δ, $(H - \mu)^{-1}$ is uniformly bounded from L^2_δ to $L^2_{-\delta}$ for $\mu \in K \times [0, 1]$. This is just a rephrasing of (b). ▮

* * *

Section XIII.6 Our discussion of what we call the Aronszajn–Donoghue theory closely follows that in W. F. Donoghue, "On the perturbation of spectra," *Comm. Pure Appl. Math.* **18** (1965), 559–579, who remarks that his results are essentially contained in N. Aronszajn, "On a problem of Weyl," *Amer. J. Math.* **79** (1957), 597–610. D. Pearson has found $V \in C^\infty$, $D^jV \to 0$ at $\pm\infty$ so that $-D^2 + V$ has purely singular continuous spectrum.

Section XIII.7 The theory of smooth operators was developed by T. Kato in two remarkable papers, "Wave operators and similarity for some non-self-adjoint operators," *Math. Ann.* **162** (1966), 258–279, and "Smooth operators and commutators," *Studia Math.* **31** (1968), 535–546. In the first paper Kato defined "H-smooth" and proved Theorems XIII.22 (in a stronger form; see Problem 49), XIII.23 (implicitly), XIII.24, XIII.25, XIII.26 (in a stronger form; see Problems 53, 54 and the discussion below), and XIII.27 (in the case $N = 2$). The second paper contains a criterion for H-smoothness if H is bounded—in case H is multiplicity free, this is the criterion of Example 4 and Problem 50—and Kato's proof of the Putnam–Kato theorem (Theorem XIII.28). Our proofs of these results are patterned on Kato's arguments.

What we call Kato's smoothness theorem appears in a stronger form in his *Math. Ann.* paper. First, he proves that $H_0 + \lambda V$ and H_0 are similar, i.e., $W(H_0 + \lambda V)W^{-1} = H_0$ for an invertible bounded operator W even when λ is complex. His proof is based on a "time-independent" formulation of scattering. Second, neither H_0 or V need be self-adjoint. What is important is that $\sigma(H_0) \subset \mathbb{R}$ and $|V|^{1/2}$ be H_0-smooth and H_0^*-smooth in the sense of the basic definition (rather than the equivalent formulations in Theorem XIII.25) and that $\sup_{\mu \notin \mathbb{R}} \| |V|^{1/2}(H_0 - \mu)^{-1}|V|^{1/2}\| < \infty$.

Weak coupling results proving that $-\Delta$ and $-\Delta + V$ are unitarily equivalent for a suitable class of small V first appeared in J. Schwartz, "Some non-self adjoint operators," *Comm. Pure Appl. Math.* **13** (1960), 609–639. Schwartz dealt with the (reduced) two-body case in $\mathbb{R}^m$ with $m \geq 3$ and proved that if $\int (1 + x^2)|D^\alpha V| \, dx < \infty$ for all $\alpha \leq m - 1$, then $-\Delta$ and $-\Delta + \lambda V$ are unitarily equivalent for λ small.

Using the Dyson series (see Section X.12), R. Prosser proved a weak coupling theorem in the two-body case in "Convergent perturbation expansions for certain wave operators," *J. Mathematical Phys.* **5** (1964), 708–713. Kato proved Theorem XIII.27 in the case $N = 2$ in his *Math. Ann.* paper; in particular, (43) was used by Kato. The Prosser and Kato proofs are based on using the series

$$\Omega^- = 1 + i\int_0^\infty V_{s_1}\,ds_1 + i^2\int_0^\infty\int_0^{s_1} V_{s_2}V_{s_1}\,ds_2\,ds_1 + \cdots$$

where

$$V_s = e^{iH_0s}Ve^{-iH_0s}$$

for $\Omega^-\varphi$, and the norm estimate

$$\|V_{s_1}V_{s_2}\cdots V_{s_n}\varphi\| = \|\,|V|^{1/2}\|\;\|\,|V|^{1/2}e^{i(s_2-s_1)H_0}|V|^{1/2}\|\cdots\|\,|V|^{1/2}e^{-is_nH_0}\varphi\|$$

Small coupling results for three-body problems were proven by Hunziker in his Boulder Lectures (see the Notes to Section XI.5) who used Prosser's techniques. He remarked that the techniques could not work for N-body systems with $N \geq 4$ because $\|\,|V_{ij}|^{1/2}e^{isH_0}|V_{kl}|^{1/2}\|$ is constant if i, j, k, l are all distinct. The idea of controlling $\int |V_{ij}|^{1/2}e^{isH_0}|V_{kl}|^{1/2}\,ds$ which appears under "Case (3)" in our proof of Theorem XIII.27 and thereby the N-body results if $N \geq 4$ is due to R. Iorio and M. O'Carroll, "Asymptotic completeness for multi-particle Schrödinger Hamiltonians with weak potentials," *Comm. Math. Phys.* **27** (1972), 137–145. It is an open conjecture that the conclusion of Theorem XIII.27 holds if $V_{ij} \in L^{m/2}$.

The theorem that H has purely absolutely continuous spectrum if there exists an A with $i[H, A] \geq 0$ appeared first in C. R. Putnam, *Commutation Properties of Hilbert Space Operators and Related Topics*, Springer-Verlag, Berlin and New York, 1967. The proof we give is from Kato's *Studia* paper.

Application of the Kato–Putnam theory to repulsive potentials appeared first in R. Lavine, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Proc. Amer. Math. Soc.* **22** (1969), 55–60. The theory was much further developed (and in particular Theorems XIII.29 and XIII.32 appear) in R. Lavine, "Commutators and scattering theory, I. Repulsive interactions," *Comm. Math. Phys.* **20** (1971), 301–323. Theorem XIII.29 appears in a slightly weaker form (an extra condition that $r\,\partial V/\partial r \ll H_0$ is added). For potentials, repulsive, central, and only $O(r^{-1-\epsilon})$, Lavine has proven the analogue of Theorem XIII.32 in "Completeness of the wave operators in the repulsive N-body problem," *J. Mathematical Phys.* **14** (1973), 376–379. Additional discussion of the two-body repulsive case can be found in M. Arai, "Absolute continuity of Hamiltonian operators with repulsive potentials," *Publ. Res. Inst. Math. Sci.* **7** (1971/72), 621–635. Our proof that $i[A, H_0] \geq 0$ follows Arai's paper.

Theorem XIII.31 and the notion of "H-smooth on Ω" are taken from R. Lavine, "Commutators and scattering theory, II. A class of one-body problems," *Indiana Univ. Math. J.* **21** (1972), 643–656.

The theory of smooth perturbations has been applied to the existence of propagators and scattering theory by E. B. Davies, "Time dependent scattering theory," *Math. Ann.* **210** (1974), 149–162, and extended to a Banach space setting in D. E. Evans, "Smooth perturbations in non-reflexive Banach spaces," *Math. Ann.* **221** (1976), 183–194.

Section XIII.8 Theorem XIII.33 is due to S. Agmon. He announced his results in "Spectral properties of Schrödinger operators," *Proc. Int. Cong. Math. of 1970*, Vol. 2, pp. 679–684, Gauthier-Villars, Paris, 1971. The details appear in S. Agmon, "Spectral properties of Schrödinger operators and scattering theory," *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* **II**, 2 (1975), 151–218.

Our approach is based on a series of lectures by Agmon together with helpful remarks by H. Epstein, J. Ginibre, and R. Lavine. Theorem XIII.33d was proven prior to Agmon in T. Kato and S. Kuroda, "Theory of simple scattering and eigenfunctions expansions" in *Functional Analysis and Related Fields*, Springer-Verlag, Berlin and New York, 1970, 99–131. That (d) follows from Agmon's a priori estimates and the theory of local smoothness is a remark of R. Lavine in the paper quoted below.

Agmon's work represents the culmination of several lines of development. The first involves proving that $\sigma_{\text{sing}}(-\Delta + V) = \emptyset$ when V is $O(|x|^{-\mu})$ at ∞ (some of the papers quoted below require additional smoothness conditions). The earliest result was for $\mu > 2$ in the paper of Ikebe quoted in the Notes to Section XI.6. This was successively improved to $\mu > \frac{3}{2}$ by W. Jäger, "Zur Theorie der Schwingungsgleichung mit variablen Koeffizienten in Aussengebieten," *Math. Z.* **102** (1967), 62–88, to $\mu > \frac{4}{3}$ in P. Rejto, "On partly gentle perturbations. III" *J. Math. Anal. Appl.* **27** (1969), 21–67, to $\mu > \frac{5}{4}$ in T. Kato, "Some results on potential scattering," *Proc. Int. Conf. on Functional Analysis and Related Topics*, Tokyo, 1969, 206–215, and to $\mu > \frac{6}{5}$ by P. Rejto in "Some potential perturbations of the Laplacian," *Helv. Phys. Acta* **44** (1971), 708–736, and by S. Kuroda (quoted below). Rejto and Kuroda both modified their methods in response to Agmon's bootstrap argument and were able to handle all $\mu > 1$. Shortly after Agmon, and independently, the case $\mu > 1$ was handled by Y. Saito, "The principle of limiting absorption for second-order differential equations with operator-valued coefficients," *Pub. Res. Inst. Math. Sci.* **7** (1972), 581–619.

A second line of development involved the idea of proving $\sigma_{\text{sing}} = \emptyset$ by a perturbation theory of maps from X to X^* where X is a Banach space imbedded in $\mathscr{H}$. We discuss such an idea in the appendix to Section XI.6. This idea was developed by J. S. Howland, "Banach space techniques in the perturbation theory of self-adjoint operators with continuous spectra," *J. Math. Anal. Appl.* **20** (1967), 22–47, and "A perturbation-theoretic approach to eigenfunction expansions," *J. Functional Analysis* **2** (1968), 1–23, and by P. A. Rejto, "On partly gentle perturbations, I–III," *J. Math. Anal. Appl.* **17** (1967), 435–462; **20** (1967), 145–187; **27** (1969), 21–67. The use of weighted L^2 spaces was first advocated (in a slightly different context) by S. Kuroda, "On the Hölder continuity of an integral involving Bessel functions," *Quart. J. Math. Oxford Ser.* **21** (1970), 71–81.

A third line of development involved the abstract theory of eigenfunction expansions of Kuroda (see the Notes to Section XI.6) and the theory of higher order elliptic operators. In fact, Agmon's theory works for a large class of operators (see Problem 70 and below). A theory with similar results was developed (partly independently of Agmon) by S. Kuroda in "Scattering theory for differential operators, I, II," *J. Math. Soc. Japan* **25** (1973), 75–104; 222–234. Let $H_0 = \sum_{|\alpha| \le 2m} a_\alpha(-iD)^\alpha$ where a_α is real. Suppose moreover that H_0 is **elliptic**, that is, $\sum_{|\alpha| = 2m} a_\alpha k^\alpha \neq 0$ for all $k \in \mathbb{R}^n$, $k \neq 0$. Let $P_1(k) = \sum_{|\alpha| \le 2m} a_\alpha k^\alpha$. A point k where grad $P_1 = 0$ is called a critical point and the value of P_1 at such a point is called a **critical value**. It can be shown that H_0 has only finitely many critical values λ_i. Let $V = \sum_{|\alpha| \le 2m} V_\alpha(x)(-iD)^\alpha$ be such that: (i) $|V_\alpha(x)| \le C_\alpha(1 + |x|^2)^{-1/2-\epsilon}$. (ii) V is formally self-adjoint, i.e., $(\varphi, V\varphi)$ is real for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (iii) For each $x \in \mathbb{R}^n$ and $k \in \mathbb{R}^n \backslash \{0\}$, $\sum_{|\alpha| = 2m}(a_\alpha + V_\alpha(x))k^\alpha \neq 0$. Then Agmon and Kuroda have proven the following generalization of Theorem XIII.33:

(a) The eigenvalues of $H_0 + V$ at noncritical values of H_0 are of finite multiplicity and can have only critical values of H_0 as limit points.

(b) If $[a, b]$ is disjoint from all critical values of H_0 and all eigenvalues of $H \equiv H_0 + V$ and if $\delta > \frac{1}{2}$, then

$$\sup_{a \le x \le b;\, 0 < y < 1} \|(H - x - iy)^{-1}\|_{\delta, -\delta} < \infty$$

(c) $\sigma_{\text{sing}}(H_0 + V) = \varnothing$.
(d) Wave operators exist and are complete.

Extensions of the Agmon–Kuroda work to a slightly larger class of potentials can be found in S. Agmon and L. Hormander, "Asymptotic properties of solutions of differential equations with simple characteristics," *J. Anal. Math.* **30** (1976), 1–38. These authors use slightly different spaces which they consider more natural.

In Agmon's original work, he does not prove or use the existence of limiting boundary values for $(H_0 - \lambda)^{-1}$ or $(H - \lambda)^{-1}$. Lemmas 6 and 7 were replaced by a limiting argument known as the "principle of limiting absorbtion." The quadratic estimates of Lemma 6 are due to Lavine.

Theorem XIII.33 is capable of generalization in two other directions. First, V need only be form compact (see Problem 71). Secondly, one can discuss the case $V = V_1 + V_2$ where $\partial V_1/\partial r$ and V_2 are $O(r^{1-\epsilon})$ at ∞. This is done by R. Lavine, "Absolute continuity of positive spectrum for Schrödinger operators with long range potentials," *J. Functional Analysis* **12** (1973), 30–54. See also T. Ikebe and Y. Saito, "The limiting absorbtion method and absolute continuity for the Schrödinger operator," *J. Math. Kyoto* **12** (1972), 513–542, and Y. Saito, "The principle of limiting absorbtion for the non-self-adjoint Schrödinger operator in $\mathbb{R}^n (N \neq 2)$" *Publ. Res. Inst. Math. Sci.* **9** (1974), 397–428.

Further developments of the Agmon–Kuroda theory appear in a series of papers by M. Schechter, "A unified approach to scattering," *J. Math. Pures Appl.* **53** (1974), 373–396; "Scattering theory for elliptic operators of arbitrary order," *Comm. Math. Helv.* **49** (1974), 84–113; "Scattering theory for second order elliptic operators," *Ann. Mat. Pura et Appl.* **55** (1975), 313–331, "Scattering Theory for Elliptic Systems," *J. Math. Soc. Japan* **28** (1976), 71–79; and "Nonhomogeneous elliptic systems and scattering," *Tohoku Math. J.* **27** (1975), 601–616.

The Agmon method has been extended to study $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ in I. W. Herbst, "Unitary equivalence of Stark Hamiltonians," *Math. Z.* **155** (1977), 55–71. Herbst proves that if $V = V_1 + V_2$ where $V_2 \in L^2(\mathbb{R}^3)$ has compact support, V_1 satisfies $|V_1(x)| \leq C(1 + (\mathbf{a} \cdot \mathbf{x})^2)^{-1/4-\epsilon}$, and $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues, then $\Omega^{\pm}(-\Delta + V + \mathbf{a} \cdot \mathbf{x}, -\Delta + \mathbf{a} \cdot \mathbf{x})$ exist and are unitary. Avron and Herbst, in their paper quoted in the notes to Section 4, give criteria under which $-\Delta + V + \mathbf{a} \cdot \mathbf{x}$ has no eigenvalues.

* * *

47. (a) Suppose the basic smoothness estimate (31) holds for a dense set of φ. Prove that for any φ, $R(\lambda \pm i\varepsilon)\varphi \in D(A)$ a.e. in λ (ε fixed, $\varepsilon \neq 0$) and that (31) holds.
    (b) Suppose that for a fixed $\varepsilon > 0$, $\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each $\varphi \in \mathscr{H}$. Prove that
$$\int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda \leq C\|\varphi\|^2$$
    for some C and all φ. (Hint: Apply the closed graph theorem to the map $\varphi \mapsto AR(\lambda + i\varepsilon)\varphi$ of $\mathscr{H}$ into $L^2(\mathbb{R}, d\lambda; \mathscr{H})$.)
    (c) Suppose that $\sup_{\varepsilon > 0} \int_{-\infty}^{\infty} \|AR(\lambda \pm i\varepsilon)\varphi\|^2 \, d\lambda < \infty$ for each φ. Prove that A is H-smooth. (Hint: Use (b) and the uniform boundedness principle.)

48. Let f be a bounded Borel function on $\mathbb{R}$ and suppose $f(H)$ is H-smooth for some self-adjoint operator H. Prove that $f(H) = 0$.

49. (a) Let H be self-adjoint and let A be H-smooth. Prove that A is $|H|^{\alpha}$-bounded for any $\alpha > \frac{1}{2}$. (Hint: Use form (3) of Theorem XIII.25 to prove that $(H^2 + 1)^{-\alpha/2}A^*$ is bounded.)

(b) Let $H = -i\, d/dx$ on $L^2(\mathbb{R})$. Prove that there exist $\varphi \in Q(H)$ that are not bounded.
(c) Find an H-smooth operator A so that A is not $|H|^{1/2}$-bounded. (Hint: Use Example 1.)

50. Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and A^*A has integral kernel K. Prove that $\|A\|_H^2 \equiv \|K\|_\infty$.

*51. Let H be multiplication by x on $L^2([\alpha, \beta], dx)$ with $\alpha, \beta \in \mathbb{R}$. Suppose that A is bounded and H-smooth. Prove that A^*A has the form (37). (Hint: First show that A^*x is in L^1 for every x with $\|A^*x\|_1 \leq C\|x\|_2$ and then use the Dunford–Pettis theorem (Problem 33 in Chapter V) to find a bounded measurable function F from $[\alpha, \beta]$ to $\mathscr{H}$, so that $(A^*x)(\lambda) = (F(\lambda), x)$.
Reference for Problem 51: Kato's *Studia Math.* paper (see the Notes to Section 7).

52. Let A and B be self-adjoint operators on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose C is A-smooth and D is a bounded operator on $\mathscr{H}_2$. Prove that $C \otimes D$ is $A \otimes I + I \otimes B$-smooth.

53. Under the hypotheses of Theorem XIII.26, prove that for any $\lambda \in \mathbb{C}$ with $|\lambda| \leq 1$, $H_0 + \lambda \sum_{i=1}^n C_i$ is a strictly m-accretive form on $Q(H_0)$, and that the associated operator H has $\sigma(H) \subset \sigma(H_0)$ and obeys $\sup\| \, |C_i|^{1/2}(H - z)^{-1} |C_j|^{1/2} \| < \infty$ for all i, j (continued in the next problem).

*54. (continued from Problem 53) Let $R(\mu)$ be the resolvent of H_0 and $R(\mu; \lambda)$ the resolvent of $H(\lambda) = H_0 + \lambda \sum_{i=1}^n C_i$. Define $W^\pm(\lambda)$ by

$$(\varphi, W_\pm(\lambda)\psi) = (\varphi, \psi) \mp \frac{\lambda}{2\pi i} \sum_{i=1}^{n} \int_{-\infty}^{\infty} (C_i^{1/2}R(\mu \pm i0)\varphi, |C_i|^{1/2}R(\mu \mp i0, \lambda)\psi)\, d\mu$$

Prove that
(a) $W_\pm(\lambda)$ are analytic in the region $|\lambda| \leq 1$.
(b) $W_\pm(\lambda)$ are invertible and $H(\lambda) = W_\pm(\lambda) H_0 W_\pm(\lambda)^{-1}$.
(c) If λ is real, $W^\pm(\lambda) = \Omega^\pm(\lambda)$.

55. Let A and H_0 be self-adjoint operators with $\operatorname{Ker}(A) = \{0\}$. Prove that, for any positive integers $n \neq m$, at most one of A^n and A^{-m} is H_0 smooth.

56. Let $V \in R$, the Rollnik class, with $\|V\|_R < 4\pi$. Prove that the wave operators provide unitary equivalences of $-\Delta$ and $-\Delta + V$ and in particular that scattering is complete.

57. (a) Let $H_n = H_0 + A_n^* B_n$ where B_n is H_0-smooth and A_n is H_n-smooth. Suppose that $\sup_n \|A_n\|_{H_n} < \infty$ and $\lim_{n \to \infty} \|B_n\|_{H_0} = 0$. Prove that $\Omega_n^\pm \equiv \text{s-lim}_{t \to \mp\infty} e^{itH_n} e^{-itH_0}$ converges to 1 *in norm*. In particular verify the norm continuity of $\Omega^\pm(\lambda) = \text{s-lim}_{t \to \mp\infty} e^{it(H_0 + \lambda C)} e^{-itH_0}$ for $\lambda \in (-1, 1)$, in the context of Theorem XIII.26.
(b) Let $V_n \to V$ in Rollnik norm. Prove that the corresponding S matrices converge strongly. (Hint: Write $V_n = W_n + Y_n$, $V = W + Y$, so that $Y_n \to Y$ in $L^1 \cap R$, $W_n \to W$ in R, and $\sup_n \|W_n\|_R < 4\pi$.)

58. (a) Let H_0 be the operator on $L^2[0, \infty)$ that is the closure of $-d^2/dx^2$ on $\{u \in C_0^\infty[0, \infty) \mid u(0) = 0\}$. Let $E \notin \sigma(H_0)$ and let

$$K_E(x, y) = E^{-1/2} \sin[\sqrt{E} \min\{x, y\}] \exp[i\sqrt{E} \max\{x, y\}]$$

where $\sqrt{E}$ is the square root with $\operatorname{Im} \sqrt{E} > 0$. Prove that

$$[(H_0 - E)^{-1}\varphi](y) = \int_0^{\infty} K_E(x, y)\varphi(y)\, dy$$

(b) $|K_E(x, y)| \le \sqrt{xy}$.
(c) Let V be a measurable function on $[0, \infty)$ with $\int_0^\infty x|V(x)|\, dx < \infty$. Then,

$$\sup_{E \notin \mathbb{R}} \| |V|^{1/2}(H_0 - E)^{-1}|V|^{1/2}\| < \infty$$

(d) If $\int_0^\infty x|V(x)|\, dx < 1$, then H_0 and $H_0 + V$ are unitarily equivalent and the wave operators are unitary equivalences.

59. Let A and H be bounded self-adjoint operators and let $R(\mu) = (H - \mu)^{-1}$. Prove that

$$|\varepsilon|\, |(R(\lambda + i\varepsilon)\varphi, [H, A]R(\lambda + i\varepsilon)\varphi)| \le \|A\|\, \|\varphi\|^2$$

and use this to prove that $(i[H, A])^{1/2}$ is H-smooth if $i[H, A] \ge 0$.

60. Let A and B be bounded self-adjoint operators and c a strictly positive real number. Prove that $i[A, B] \ge cI$ is impossible by:
(a) using the theory of smooth perturbations;
(b) direct computation (look at $e^{iAt}Be^{-iAt}$).

61. Extend the Kato–Putnam theorem to the case where H is unbounded and $i[H, A] > 0$ means that $i(A\varphi, H\varphi) - i(H\varphi, A\varphi) > 0$ for all $\varphi \in D(H)$, $\varphi \ne 0$.

†62. Suppose that $f(t)$ is a Banach-space-valued uniformly continuous function on $\mathbb{R}$. Suppose also that $\int_{-\infty}^{\infty} \|f(t)\|^p\, dt < \infty$ for some $p < \infty$. Suppose that f is strongly differentiable with a uniformly bounded derivative. Conclude that $\lim_{t \to \infty} f(t) = 0$.

†63. Fill in the computations in the proof of Theorem XIII.29.

†64. Fill in the details of the proof of Theorem XIII.32.

65. By iterating the proof of (a) in Theorem XIII.33, prove that if $H_0\varphi = \lambda\varphi - V\varphi$ with $\lambda > 0$, then $\varphi \in L_\delta^2$ for all δ.

†66. (a) Prove that $(-\Delta - \mu)^{-1}$ is bounded from L_δ^2 to L_δ^2 for any δ and any $\mu \in \mathbb{C}\backslash\mathbb{R}$. (Hint: Prove it for $\delta > 0$ inductively in $[0, 1]$, $(1, 2]$, $\ldots$.)
(b) Complete the proof of Lemma 1 in Section 8.
(c) Prove that $(-\Delta + 1)^{-1}\, \partial/\partial x_i$ is a bounded map from L_δ^2 to L_δ^2 for any δ.

†67. Verify the bound (62).

68. Let $\delta > n + \frac{1}{2}$. Prove that, for any $b > a > 0$, there is a constant C so that

$$\|(-\Delta - \lambda - i0)^{-n}\varphi\|_{-\delta} \le C\|\varphi\|_\delta$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^m)$ and all $\lambda \in [a, b]$.

69. Let $\|A\|_{\delta, -\delta}$ denote the norm of A as a map of L_δ^2 to $L_{-\delta}^2$. Let $\delta > \frac{1}{2}$. Prove that for any $\alpha < \min\{1, \delta - \frac{1}{2}\}$, $(H_0 - \mu - i0)^{-1}$ is Hölder continuous of order α as an $\mathcal{L}(L_\delta^2, L_{-\delta}^2)$-valued function of μ, i.e., for any $\mu > 0$, there is a C and an ε so that

$$\|(H_0 - \mu' - i0)^{-1} - (H_0 - \mu - i0)^{-1}\|_{\delta, -\delta} \le C|\mu - \mu'|^\alpha$$

if $|\mu - \mu'| < \varepsilon$.

*70. Let V be an Agmon potential. Let $a_1, \ldots, a_n$ obey $\sum_{i=1}^{n} \partial_j a_j = 0$ (distributional sense) with $|a_j(x)| \le C_j(1 + |x|^2)^{-1/2-\epsilon}$. Let

$$H = -\Delta + 2i \sum_{j=1}^{n} a_j \, \partial_j + \sum_{j=1}^{n} a_j^2 + V$$

Prove that $\sigma_{\text{sing}}(H) = \emptyset$ and that $\Omega^{\pm}(H, H_0)$ exist and are complete. (Hint: Develop a theory paralleling Theorem XIII.33.)

*71. Suppose $V(x) = (1 + |x|^2)^{-1/2-\epsilon} W(x)$ where W is a form relatively compact perturbation of $-\Delta$. Prove that Theorem XIII.33 remains valid.

List of Symbols

Superscripts refer to page numbers in other volumes. The boldface convention is discussed on page 7.

C	the complex numbers	
$C(X)$		102^1
$C_0^\infty(\mathbb{R}^n)$		145^1
$\mathscr{C}_{\alpha,\beta}$		96
$d\Gamma(A)$		302^1, 208^2
$\mathscr{D}_{L\infty}$		67
$D(\cdot)$	(domain)	249^1
$\mathscr{D}(\mathbb{R}^n)$, $\mathscr{D}(\Omega)$		147^1
$\mathscr{D}'(\mathbb{R}^n)$, $\mathscr{D}'(\Omega)$		148^1
D^α		2^2
$D(\alpha)$		84
$D \lhd D'$		89
$D' * D$		91
EBFM		4
$\mathscr{E}$		99
$E_\Omega(A)$		28
$f(k)$		117
$f(k, \theta)$		111
$f(E, \cos\theta)$		127
$f(A)$	(continuous functional calculus)	222^1
$\hat{f}$, $\mathscr{F}$	(Fourier transform)	1^2

$\check{f}$, $\mathscr{F}$	(inverse Fourier transform)	1^2
$\mathscr{F}(\mathscr{H})$		53^1
$F_\perp(x)$		175
$F_\parallel(x)$		175
$G_0(x, y)$		102, 103
$G(x, y)$		102, 103
$G_{\Gamma;D}$		206
$G_{\Gamma:N}$		206
$\boldsymbol{k}$		295
$\mathscr{H}$		39^1
$\mathscr{H}_{\mathrm{pp}}$, $\mathscr{H}_{\mathrm{ac}}$, $\mathscr{H}_{\mathrm{sing}}$		230^1
$\mathscr{H}_{\mathrm{asym}}$		85
$\mathscr{H}_\alpha$		85
$\mathscr{H}_\pm^2$		219
$\mathscr{H}_{\substack{\mathrm{in}\\\mathrm{out}}}$		321
H_0	(free Hamiltonian)	55^2
H_α		85
H_{asym}		85
$H^\otimes$		290
$H(C_\ell)$, $\tilde{H}(C_\ell)$		79

H_D		79
$\mathcal{I}_p$		207^1, 208^1, 41^2, 47
$\mathcal{I}_p(\mathcal{H}_1, \mathcal{H}_2)$		36
I_D		79
Ker		185^1
KLMN		167^2
ℓ_p		69^1
$L^p(X, d\mu)$		68^1
$L^2(X, d\mu : \mathcal{H}')$		40^1
L^p_{loc}	(functions locally L^p)	
L^2_δ	(weighted L^2)	47
L^p_w	(weak L^p)	30^2
$L^r + L^s$		165^2
$\mathcal{L}(\mathcal{H})$		182^1
$\mathcal{L}(X, Y)$		69^1
$\mathcal{M}(B)$		23
$p(D)$		45^2
$P_\Omega(A)$, P^A_Ω		234^1
P_{cont}		341
$\mathcal{P}_n$		323
$\mathbb{R}$		the real numbers
R	(Rollnik class)	99
$R_{\alpha\beta}$		95
Ran		185^1
$R(\lambda + i\mu)$, $R_\lambda(T)$	(resolvent)	188^1
R_0, $R_{\Gamma;\mathrm{N}}$, $R_{\Gamma;\mathrm{D}}$, $\tilde{R}_{\partial\mathrm{B}\cup\Gamma;\mathrm{N}}$		203
supp		139^1, 17^2
S	(scattering operator)	see index
$\hat{S}$, $\tilde{S}$		213
$S(E)$		123
$S(k, k')$		108
$\mathcal{S}(\mathbb{R}^n)$		133^1
$\mathcal{S}'(\mathbb{R}^n)$		134^1
$\mathrm{tr}(\cdot)$		207^1, 208^1
TVEV		323
$T(k, k')$		107
$T(E)$		127
VEV		323
$W_m(\Omega)$	(Sobolev spaces)	50^2
x^α		2^2
$\Gamma(T)$	(operator graph)	250^1
$\Gamma(A)$		309^1, 208^2
$d\Gamma(A)$		302^1, 208^2
$\delta_\ell(E)$		129
Δ	(symmetric set difference)	
Δ	(Laplacian on $\mathbb{R}^n$)	
$\Delta^\Omega_{\mathrm{D}}$	(Dirichlet Laplacian)	263^4
$\Delta^\Omega_{\mathrm{N}}$	(Neumann Laplacian)	263^4
$\kappa(X)$		111^1

$\rho(T)$		188^1
$\sigma(T)$		188^1
σ_x, σ_y, σ_z, $\sigma_\pm$	(Pauli matrices)	287
σ_{pp}, σ_{cont}, σ_{ac}, σ_{sing}		231^1
σ_{disc}		236^1
σ_{ess}		236^1, 15
σ	(cross section)	15, 111
$d\sigma/d\Omega$	(differential cross section)	15
Σ_{in}, Σ_{out}		3
Σ_0		8
$\tau_F(k)$		116
$\dot{\mathcal{T}}$		86
$\mathcal{T}_\alpha$		85
χ_A		2^1
$\Omega^\pm$		8
$\Omega^\pm(A, B)$		17
$\Omega^\pm(A, B, J)$		24
$\Omega^\pm_\alpha$		85
$\Vert \cdot \Vert_p$	(functions)	68^1
$\Vert \cdot \Vert_p$	(operators)	41^2
$\Vert \cdot \Vert_R$	(Rollnik norm)	99
$\Vert \cdot \Vert_\infty$	(functions)	67^1
$\Vert \cdot \Vert_\infty$	(operators)	81^2
$\Vert \cdot \Vert_\delta$	(weighted L^2)	438
$\Vert \cdot \Vert_{op}$	(operator norm)	9^1
$\oplus$		40^1, 78^1
$\otimes$	(measures)	26^1
$\otimes$	(Hilbert spaces)	49^1
$\otimes$	(functions)	141^1
$\otimes$	(operators)	299^1
$\leq$	(operators)	75^4, 85^4, 269^4
$\lhd$		89
$-$	(closure)	92^1
$^\circ$, $^{\mathrm{int}}$	(interior)	92^1
$*$	(adjoint)	187^1
$*$	(dual space)	72^1
$*$	(convolution)	6^2, 7^2
$*$	(common cluster refinement)	91
$\xrightarrow{\Vert\cdot\Vert}$, $\xrightarrow{w}$, $\xrightarrow{s}$		182^1, 183^1
$\vert \cdot \vert$	(absolute value of an operator)	196^1
$\perp$	(orthogonal complement)	41^1
$\setminus$	(set difference)	1^1
$/$	(quotient)	78^1, 79^1
$\restriction$	(restriction)	2^1
$<\cdot, \cdot>$	(ordered pair)	1^1
$(\cdot, \cdot)$	(inner product)	36^1

Index

Superscripts on page numbers refer to other volumes.

A

Abelian limits, 105
Absolute value of an operator, 196^1
Absolutely continuous subspace, 230^1
Acoustical scattering, 184–243
Action, 279
Adjoint, Banach space, 185^1
Adjoint, Hilbert space, 186^1
Adjoint, unbounded operator, 252^1
Admissible function, 29
Agmon–Kato–Kuroda theorem, 439
Agmon potential, 439
Analytic Fredholm theorem, 201^1
Analytic function, vector-valued, 189^1–190^1
Analytic S-matrix hypothesis, 96
Antibound states, 144
Approximate identity, 251^1, 9^2
Associated Legendre functions, 151
Asymptotic completeness, 4
  weak, 3
Asymptotic,
  Hilbert space, 85
  left inverse, 35
Asymptotically equivalent, 35
Atomic coordinates, 78
Avron–Herbst theorem, 61
Axiomatic quantum field theory, 62^2

B

Baire measure, 105^1, 110^1
Banach space, 67^1
Belopol'skii–Birman theorem, 36
Bessel's equation, 153
Birman's theorem, 28
B.L.T. theorem, 9^1
Bogoliubov transformation, 316
Boldface convention, 7
Boltzmann equation, 244
Born amplitude, 109

Born series, 109
Bounded operator, 8^1
Breakup processes, 77
Broken invariance, 282

C

Canonical ellipse, 151
Canonical form for compact operators, 203^1
Capture processes, 76
Cauchy sequence, 5^1
Central force, 13
Central potentials, 121–168
  almost, 175
Chain rule, 18
Channel, 84
  eigenenergies, 84
  embedding, 85
  Hamiltonian, 85
  Hilbert space, 85
  wave operators, 85
Charge,
  conformal, 275
Charge operator, 300
Charged free scalar Boson field, 300
Closed graph theorem, 83^1
Closed operator, 250^1
Closed quadratic form, 277^1
Cluster decomposition, 79
Cluster Hamiltonian, 79
Cluster properties,
  of TVEV, 324
  spatial, 75, 93–96
Clustered channel wave operators, 82
Clustered Jacobi coordinates, 79
Commuting (unbounded) operators, 271^1–272^1
Compact operators, 199^1, *see also* Relatively compact; Relatively form compact
  determinant, 323^4, 382^4
  general theory, 198^1–206^1, 316^4–338^4
  Hilbert-Schmidt, 210^1
  ideal theory, 41^2–44^2
  resolvent, 244^4–260^4
  trace class, 206^1–213^1
Compact support
  distributions, 319^1, 178^1, 17^2
  functions, 111^1
Complete wave operators, 19, 35, 88
  asymptotically, 4, 18
  weakly asymptotically, 3, 18
Cone property, 204
Conformal charge, 275, 285
Conformal transformation, 285
Conserved current, 281
Continuous functional calculus, 222^1
Contraction, 151^1, 235^2
Convolution
  distributions, 7^2
  functions, 6^2
Cook–Hack theorem, 56
Cook's method, 20
Coordinates,
  atomic, 78
  Jacobi, 78
  clustered Jacobi, 79
Core, 256^1
Critical value, 449
Cross-section measure, 15
Cumulants, 381
Currents,
  conserved, 278–285

D

Decomposable operator, 123
Decomposition,
  of a channel, 93
Deficiency indices, 138^2
Differential cross section, 15
Dilation current, 282
Dilation transformation, 282
Direct sum
  of Banach spaces, 78^1
  of Hilbert spaces, 40^1
Dirichlet Green's function, 206
Dirichlet Laplacian, 263^4
Discrete spectrum, 236^1, 13^4
Dispersion relations, 116
Distributions
  compact support, 139^1, 178^1, 17^2
  tempered, 134^1
Dollard–Friedman theorem, 161
Domain
  analytic function, 189^1
  form, 276^1

  function, 2^1
  unbounded operator, 249^1
Dominated convergence theorem, 17^1, 24^1
Dual space, 43^1, 72^1
Dynamical cut, 145
Dyson expansion, 282^2

E

EBFM S-matrix, 4
Eigenfunction expansions, 96
  auxiliary space method, 122
Eigenvalue, 188^1
Eigenvector, 188^1
Elastic scattering, 76
Electric field scattering, 59
Elliptic operator, 449
Elliptic regularity, 49^2
Embedding transformation, 86
Energy-momentum tensor, 282
Energy representation, 123
Energy shell, 108
Enss potential, 332
Enss's Theorem, 333
Equivalent measures, 215
Essential support of an operator, 393
Essentially self-adjoint, 256^1
Euler–Lagrange equation, 278
Exceptional set, 99
Excitation collisions, 77
External field scattering, 293–316
Extension of an operator, 250^1

F

False poles, 145
Fatou's theorem, 233
fiber, 123
Finite mean free path, 250
First resolvent formula, 191^1
Fock space, 53^1
Form, see also Quadratic forms
  core, 277^1
  domain, 276^1
    of operator, 277^1
Forward scattering amplitude, 117
Fourier inversion theorem, 3^2
Fourier transform, 1^2
Free Green's function, 102, 208
Free Hamiltonian, 85
  charged scalar field, 299
  nonrelativistic quantum mechanics, 55^2
Friedrichs' extension, 177^2
Functional calculus, 222^1, 225^1, 245^1, 263^1, 286^1–287^1
Functions of rapid decrease, 133^1

G

Generalized wave operators, 17
Generator
  group, 268^1
  semigroup, 237^2, 246^2
Graph, 83^1, 250^1
Green's functions, 102, 103, 206
  trace class properties, 203
  Dirichlet, 206
  Neumann, 206

H

H-smooth, 412
Haag–Ruelle theory, 317
Hack's theorem, 82
Hahn–Banach theorem, 75^1–77^1
Hamilton–Jacobi equation, 183
Hamiltonian, 303^1
  free, 55^2, 220^2
  time dependent, 109^2
Hausdorff–Young inequality, 11^2
Heisenberg model, 286
Heisenberg picture scattering operator, 307
Hermitian operator, *see* Symmetric operator
Hilbert–Schmidt operators, 210^1
Hilbert–Schmidt theorem, 203^1
Hilbert space, 36^1
Hölder's inequality, 68^1, 34^2
  matrices, 385^4
  operators, 41^2
Hughes–Eckart terms, 78
Huygens' principle, 221
HVZ theorem, 121^4

I

Impact parameter, 14
Incoming spectral representation, 219
Incoming subspace, 211
Incoming translation representation, 212
Infinitesimal generator
  group, 268^1
  semigroup, 237^2, 246^2
Infrared problem, 381
Intercluster potential, 79
Internal symmetry, 404
Interpolation theorems, 32^2
Invariance principle, 31
Inverse Fourier transform, 1^2
Iorio–O'Carroll theorem, 424

J

Jacobi coordinates, 78
Jauch S-matrix, 322
Jost equation, 137
Jost function, 140
Jost solutions, 139
  for oscillatory potentials, 155

K

K-system, 369
Kato–Birman theory, 22
Kato–Rosenblum theorem, 26
Kato's smoothness theorem, 422
Kinematical cut, 145
Kohn variational principle, 147
Kupsch–Sandhas theorem, 21
Kuroda–Birman theorem, 27

L

L^p inequalities, 32^2
Laplacian
  Dirichlet, 263^4
  Neumann, 263^4
  on $\mathbb{R}^n$, 54^2
Lavine's theorem, 429
Lax–Phillips method, 210–241
Least action, 279
Left-hand cut, 145
Legendre's equation, 149
Legendre polynomials, 149
Lehmann ellipse, 119
Levinson's theorem, 142
Lippman–Schwinger equation, 98
Local smoothness, 433
Long-range potentials, 169–183
Lorentz inversion, 283

M

Magnetic field scattering, 66
Magnetic spin waves (magnons), 286
Mass gap, 319
Measurable, weakly and strongly, 64^1, 115^1–117^1
Measurable functions, sets, 14^1–16^1, 19^1–24^1, 104^1–111^1
Measurable unbounded operator-valued function, 283^4
Measure, 19^1–25^1, 104^1–111^1
Meromorphic Fredholm theorem, 107^4
Monotone convergence theorem, 17^1, 24^1
  for nets, 106^1
Mutually subordinate operators, 28

N

Neumann Green's function, 206
Neumann Laplacian, 263^4
Neutron transport equation, 245
Noether's theorem, 278, 279
Norm, 8^1
  operator, 9^1
Norm resolvent sense, convergence in, 284^1–291^1
Number operators, 299

O

On-shell T-matrix, 108
One-parameter unitary group, 265^1
Open channels, 124
Operator
  adjoint
    Banach space, 185^1

    - Hilbert space, 186^1
    - unbounded, 252^1
  - bounded, 8^1
  - compact, 199^1
  - compact resolvent, 244^4
  - contraction, 235^2
  - decomposable, 281^4
  - dilation, 183^4
  - elliptic, 112^2, 346^4
  - energy (Hamiltonian), 303^1
  - general theory, 81^1–84^1, 182^1–216^1
  - Hamiltonian, 303^1
  - Hermitian, *see* Operator, symmetric
  - Hilbert–Schmidt, 210^1
  - ideals, 41^2–44^2
  - infinitesimally form small, 168^2
  - infinitesimally small, 162^2
  - locally smooth, 433
  - momentum, 304^1, 63^2
  - non-self-adjoint, 316^4–338^4
  - norm, 9^1
  - normal, 246^1
  - positive, 195^4
  - positivity improving, 201^4
  - positivity preserving, 201^4
  - relatively bounded, 162^2
  - relatively compact, 113^4
  - relatively form bounded, 168^2
  - relatively form compact, 369^4
  - resolvent, 188^1, 253^1
  - Schrödinger, 79^4
  - self-adjoint, 187^1, 255^1
  - smooth, 411–437
  - symmetric, 255^1
  - tensor product, 299^1
  - topologies, 182^1–185^1, 283^1–295^1, 41^2–44^2, 268^2–273^2
  - trace class, 207^1–210^1
  - unbounded, general theory, 249^1–312^1
- Optical scattering, 197
- Optical theorem, 111
- Outgoing spectral representation, 219
- Outgoing subspace, 211
- Outgoing translation representation, 212

P

- Paley–Wiener theorems, 16^2, 17^2, 18^2, 23^2, 109^2
- Parseval's relation, 45^1–46^1
- Partial wave expansion, 128
- Partial wave scattering amplitudes, 128
- Partial wave unitarity, 130
- Partition, 323
- Pauli matrices, 287
- Pearson's counterexample, 71
- Pearson's theorem, 24
- Periodic potentials, 279^4
- Phase shifts, 129
- Phase space, 5
- Plancherel theorem, 10^2
- Polar decomposition, 197^1, 297^1
- Polarization identity, 63^1
- Positive commutators, 427
- Positive operator, 195^1
- Principle of least action, 279
- Principle of uniform boundedness, 81^1, 132^1
- Product formula, 295^1–297^1, 245^2
- Projection, 187^1
- Projection valued measure (p.v.m.), 234^1–235^1, 262^1–263^1
- Putnam–Kato theorem, 427

Q

- Quadratic forms, 276^1
  - closed, 277^1
  - form core, 277^1
  - form domain, 276^1
  - Friedrichs' extension, 177^2
  - infinitesimally bounded, 168^2
  - positive, 276^1
  - relatively bounded, 168^2
  - relatively compact, 369^4
- Quantum scattering,
  - central potentials, 121–168
  - dispersion relations, 116–120
  - eigenfunction expansions, 96–115
  - long-range potentials, 169–183
  - *N*-body, 75–95
  - two-body, 54–74
- Quantum field scattering,
  - external field, 293–316
  - Haag–Ruelle theory, 317–330

R

- RAGE theorem, 341

Rearrangement collisions, 77
Reduction of the S-matrix, 121
Reduction formulas, 381
Refinement, 89
Regular equation, 136
Regular pair, 244
Regular operator, 234
Regular solution, 137
Regular wave packet, 42
Relatively bounded, 162^{2}
Relatively compact, 113^{4}
Relatively form bounded, 168^{2}
Relatively form compact, 369^{4}
Resolvent, 188^{1}, 253^{1}
Resolvent set, 188^{1}, 253^{1}
Resonance poles, 144
Restricted cone property, 204
Riemann–Lebesgue lemma, 10^{2}
Riesz's lemma, 43^{1}
Right-hand cut, 145
Rollnik class, 99
Rosenberg–Spruch bound, 148

S

S-matrix, S-Operator, *see* Scattering operator
Scattering amplitude, 111, 127
  forward, 117
Scattering angle, 14
Scattering length, 136
Scattering operator,
  external quantum fields, 307
  Lax-Phillips method, 212
  quantum fields, 322
  quantum mechanics, 73, 87
    cluster properties, 93
Scattering theory
  acoustical, 184–243
  classical particles, 5–15
  Enss's method, 331–343
  external quantum fields, 293–316
  Hilbert space methods, 16–36
  Lax–Phillips method, 210–242
  long-range, 169–183
  nonlinear wave equations, 252–277
  on C^*-algebras, 382–384
  optical, 184–243
  quantum mechanics,
    2-body, 54–74
    N-body, 75–95
    central potentials, 121–168
    dispersion relations, 116–120
    eigenfunction expansions, 96–115
    long-range, 169–183
  spin waves, 285–292
Scattering transformation, 3, 13
Schrödinger equation, 303^{1}
Schrödinger integral equation, 136, 137
Schwartz space, 133^{1}
Schwarz inequality, 38^{1}
Self-adjoint operator
  bounded, 187^{1}
  unbounded, 255^{1}
Semibounded operator, 137^{2}
Semibounded quadratic form, 276^{1}
Semicomplete wave operator, 35
Semigroup
  contraction, 235^{2}
  holomorphic, 248^{2}, 252^{2}
  hypercontractive, 258^{2}
  infinitesimal generator, 237^{2}, 246^{2}, 248^{2}
  L^p-contractive, 255^{2}
  strongly continuous, 235^{2}
Singular continuous spectrum,
  absence of, 406–453
Smooth boundary, 209
Smooth perturbations, 411–437
Smooth solutions of the Klein–Gordon equation, 43
Sobolev inequality, 31^{2}, 113^{2}
Sobolev lemma, 52^{2}
Sobolev spaces, 50^{2}, 253^{4}
Source, 281
Spatial cluster properties, 93
Spectral mapping theorem, 222^{1}, 109^{4}, 181^{4}–183^{4}
Spectral measures, 228^{1}
  associated with a vector, 225^{1}
Spectral projections, 234^{1}
Spectral theorem
  functional calculus form, 225^{1}, 263^{1}
  multiplication operator form, 227^{1}, 260^{1}
  p.v.m. form, 235^{1}, 263^{1}–264^{1}
Spectrum, 188^{1}
  absolutely continuous, 231^{1}
  approximate point, 178^{4}
  asymptotically in a set, 46^{4}
  continuous, 231^{1}

  continuous singular, 231^1
  discrete, 236^1, 13^4
  essential, 236^1
  point, 188^1, 231^1
  residual, 188^1
Spherical Bessel functions, 153
Spin up, 287
Spin down, 287
Starlike, 209
Stationary methods, 354
Stationary phase, 37
Stone's formula, 237^1
Strong operator topology, 182^1
Strong resolvent sense, convergence in, 284^1–291^1
Strongly continuous semigroup, 235^2
Strongly continuous unitary group, 265^1
Strongly semibounded local perturbation of $-\Delta$, 67
Subchannels, 92
Subcritical, 249
Subordinate operators, 28
Support of a distribution, 139^1, 17^2
  singular, 88^2
Symmetric operator, 255^1
Symmetric quadratic form, 276^1
Symplectic transformation, 376

T

T-matrix, 107
Tensor product
  Hilbert spaces, 49^1
  operators, 299^1
    spectrum of, 177^4
Threshold for channel α, 124
Time delay, 14
Time-dependent Schrödinger equation, 61
Time-zero fields, 300
Trace class, 207^1–210^1
Transport equation, 243
Trotter product formula, 295^1–297^1, 245^2
Truncated cone, 204
Truncated vacuum expection value, 323
Twisting trick, 241

U

Uniform boundedness principle, *see* Principle of uniform boundedness
Uniform operator topology, 182^1
Unitarity relation for the T-matrix, 110
Unitarity cut, 145
Unitary operator, 39^1
Ursell functions, 381

V

Variable phase equation, 133
von Neumann's theorem, 268^1, 143^2, 180^2
von Neumann's uniqueness theorem, 217, 275^1

W

Wave operators,
  complete, 35
  generalized, 17
  semicomplete, 35
Weak asymptotic completeness, 3
Weak-L^p, 30^2
  inequalities, 32^2
Weak topology, 93^1, 111^1
Weakly coupled quantum systems, 421
Weakly measurable (vector-valued) function, 114^1
Weighted L^2 space, 76^2, 438
Wiener's theorem, 340

Y

Young's inequality, 28^2
Yukawa potential, 120
  generalized, 120